REMARKS

Reconsideration is respectfully requested. Claims 1, 4, 6, 9, 10, and 18-24 are pending. Claims 2-3, 5, 7-8, and 11-17 are canceled. New claim 24 is added. Claims 1, 4, 9 and 19 are amended. Cancellation and amendment of the claims does not affect inventorship.

Applicants have not dedicated or abandoned any unclaimed subject matter and moreover have not acquiesced to any rejections made by the Patent Office. Applicants reserve the right to pursue prosecution of any presently excluded claim embodiments in future continuation and/or divisional applications.

Claim Amendments

Claims 1, 4, 9 and 19 are amended. New claim 24 has been added. Support is found in the specification, for example, in paragraphs [00178] and [00183].

Objections to the Specification

The Examiner has objected to the Specification because of certain informalities, each of which are addressed separately below:

Firstly, the specification is objected to because of the inappropriate use of SEQ ID NOs and number of residues that do not correspond to the SEQ ID NOs. The Examiner specifically cites to paragraph [00180] in connection with the objection. Applicants respectfully direct the Examiner's attention to the Amendment in Response to Official Action filed on June 30, 2006, wherein Applicants amended several portions of the Specification, and specifically requested that paragraph [00180] be deleted. Thus, the objection raised by the Examiner with respect to paragraph [00180] is moot in light of its deletion.

Secondly, the Examiner refers to informalities in Example 2, i.e., paragraph [00183] of the Specification. The Examiner is referred to the Amendment in Response to Official Action filed on June 30, 2006, wherein Applicants amended paragraphs [00178] and [00183]. The amendment specifically states that SEQ ID NO:2 comprises a coding sequence for a N-terminal His-tag coupled to full length IspA, and that SEQ ID NO:2 is expressed in the pSX28 vector to generate a fusion protein of the full length IspA with a non-cleavable amino-terminal six histidine tag, i.e., SEQ ID NO:1. The foregoing amendment in conjunction with the deletion of paragraph [00180] renders the objection moot.

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Thirdly, the Examiner has raised an objection with respect to a typographical error in the Oath and Declaration concerning the spelling of the first inventor's name. The first inventor's name is correctly spelled as Alexei Brooun in the Oath and Declaration; whilst being incorrectly spelled in the Hosfield et al. (2004) publication. Thus, there is no error in the Oath and Declaration.

In light of the above arguments, the Examiner is requested to withdraw the objections to the Specification.

Objections to the Drawings

In response to the objection to the drawings raised by the Examiner, Applicants have submitted corrected annotated and replacement drawing sheets for Figure 3, in conjunction with this paper.

Claim Rejection Under 35 U.S.C. § 112

<u>Indefiniteness</u>

Claims 1, 4 and 16 are rejected for failing to particularly and distinctly claim the subject matter which applicant regards as the invention. Claim 16 has been canceled and its claim limitation is now incorporated in claims 1 and 4. Claims 1 and 4, as amended, are directed to a composition comprising a protein in crystalline form, wherein the protein consists of residues 1-314 of SEQ ID NO:1, and wherein the protein crystal has a crystal lattice in a P4₁22 space group and unit cell dimensions, +/- 5%, of a=88.80Å b=88.80Å and c=174.99Å, $\alpha=\beta=\gamma=90$ (emphasis added). Applicants believe that the scope of claims 1 and 4 as currently recited are clear on their face, and therefore respectfully request the withdrawal of the instant rejection.

Written Description and Enablement

Claims 1,4,6, 9, 10, 16 and 18-23 stand rejected under 35 U.S.C. § 112, first paragraph as failing to comply with the written description and enablement requirement. Applicants respectfully traverse.

Claim 16 has been cancelled, thereby rendering the rejections with respect to this claim moot.

Applicants respectfully direct the Examiner to M.P.E.P. 2163, which states:

The written description requirement for a claimed genus may be satisfied through sufficient description of a representative number of species by actual reduction to practice.

The Examiner states that:

While the structure and function of one species of said genera of IspA are disclosed in the specification, the common structural characteristics of species that define said genera are not described.

Applicants respectfully disagree. Claim 1 as amended recites a protein crystal having a crystal lattice in a P4₁22 space group and unit cell dimensions, +/- 5%, of a=88.80Å b=88.80Å and c=174.99Å, $\alpha=\beta=\gamma=90$. Thus, it claims a genus method to grow this specific crystal of a protein. As stated in M.P.E.P. 2163:

A "representative number of species" means that the species which are adequately described are representative of the entire genus.

. . . .

What constitutes a "representative number" is an inverse function of the skill and knowledge in the art. Satisfactory disclosure of a "representative number" depends on whether one of skill in the art would recognize that the applicant was in possession of the necessary common attributes or features of the elements possessed by the members of the genus in view of the species disclosed.... Description of a representative number of species does not require the description to be of such specificity that it would provide individual support for each species that the genus embraces.

Moreover, as the Examiner can appreciate, at the beginning of this new millennium, the time the instant application was filed, "the skill and knowledge in the art" required for growing crystal had come a long way from the early age of crystallography, or even a decade before then. Kits for large scale screening were widely commercially available, and methods and equipments for robotic large scale screening have been developed by several entities. Due to these developments, large scale screening with minimal amount of protein for conditions to grow crystals became routine, particularly in the industry.

A simple search on Google Scholar for references relating to protein crystallization methods yielded in excess of 30,000 hits most of which had a publication date prior to the filing date of the instant application in 2003. A sampling of the references is provided below. Therefore, it is quite clear that the level of skill in the art was high, with respect to crystallization methods, at the time the application was filed. Hence, a skilled artisan would have been more than capable of arriving at the conditions for crystallization of a protein consisting of "residues 1-314 of SEQ ID NO:1."

List of References

High-throughput protein crystallization - RC Stevens - Curr. Opin. Struct. Biol, 2000

Overview of Protein Crystallization Methods- PC Weber - Methods in enzymology, 1997

Comparative studies of protein crystallization by vapour-diffusion and microbatch techniques - NE Chayen - Acta Crystallogr D Biol Crystallogr, 1998

An approach to rapid protein crystallization using nanodroplets - DC Uber, EW Cornell, RA Nordmeyer, WF Kolbe, J Jin - J Appl Crystallogr, 2002

An automated system for micro-batch protein crystallization and screening - NE Chayen, PD Shaw Stewart, DL Maeder, DM Blow - Journal of Applied Crystallography, 1990

Protein crystallization for genomics: towards high-throughput optimization techniques - NE Chayen, E Saridakis - Acta Crystallographica Section D Biological Crystallography, 2002

Protein Crystallization - SD Durbin, G Feher - Annual Review of Physical Chemistry, 1996

System for Evaluating Protein Crystallization Conditions by Microbatch and Vapor-Diffusion Methods - B Zheng, JD Tice, LS Roach, RF Ismagilov - Angewandte Chemie International Edition, 2004

Principles of Protein X-Ray Crystallography- J Drenth - 1999

Screening of protein crystallization conditions on a microfluidic chip using nanoliter-size droplets - B Zheng, LS Roach, RF Ismagilov - J Am Chem Soc, 2003

Protein interactions and crystallization- DF ROSENBAUM, CF ZUKOSKI - Journal of crystal growth, 1996.

Protein Crystallization: Micro Techniques Involving Vapor Diffusion- DR Davies, DM Segal - Methods Enzymol, 1971

As such, at the time the instant application was filed, "the skill and knowledge in the art" had grown into a stage that it was not necessary to disclose each and every condition, foreseeable or unforeseeable, to meet the ""representative number" requirement. Description of a representative number of conditions to grow the claimed specific crystal does not require the description of such specificity each growing condition. The wide range of crystallization conditions disclosed by the present invention is sufficient to provide guidance to further explore for new conditions to grow the claimed crystal.

As such, at the time the instant application was filed, "the skill and knowledge in the art" had grown into a stage that it was not necessary to disclose each and every condition, foreseeable or

unforeseeable, to meet the ""representative number" requirement. Description of a representative number of conditions to grow the claimed specific crystal does not require the description of such specificity each growing condition. The wide range of crystallization conditions disclosed by the present invention is sufficient to provide guidance to further explore for new conditions to grow the claimed crystal.

Applicants further submit that a sufficient "representative number" of conditions - the conditions to grow the specific crystal as recited in claim 6- have been provided by the instant application. The specification discloses that the Applicants have undertaken "systematic broad screening crystallization trials on an IspA complex using the sitting drop techniques" to obtain conditions that appear to produce precipitate and/or crystals. These conditions are used for fine screening for optimal conditions. *See* paragraphs [0086] and [0087]. These experiments led to a thorough understanding of how crystallization conditions affect IspA crystallization, and a series of crystallization conditions were identified that maybe used to for crystals comprising IspA. These conditions are summarized in Table 8. The specification further discloses in details one of the crystals obtained under one of the disclosed conditions. *See* Example 2. Therefore, the Applicants have disclosed a range of conditions that can be used to grow the claimed specific crystal.

Thus, at the time of the filing, Applicants not only were in possession of the claimed genus method, but also provided sufficient guidance to enable a skilled artisan to practice the claimed method without undue experimentation. As such, the rejection is improper and should be withdrawn.

CONCLUSION

Applicants respectfully submit that the claims are now in condition for allowance and early notification to that effect is respectfully requested. If the Examiner feels there are further unresolved issues, the Examiner is respectfully requested to phone the undersigned at (415) 442-1000.

Respectfully submitted,

Dated:

Customer Number: 67374 Morgan, Lewis & Bockius LLP

One Market, Spear Street Tower San Francisco, CA 94105

Telephone: (415) 442-1000 Facsimile: (415) 442-1001 By:

Lekha Gopalakrishnan, Reg. No. 46,733

Filed Under 37 C.F.R. § 1.34

On behalf of:

Robin M. Silva, Reg. No. 38,304



FIGURE 3<u>AA</u>

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	E	F	G	Н	I	J
1	N	MET	Α	16	65.564	50.628	-5.933	1.00	45.23
3	CA	MET	Α	16	65.166	51.178	-7.255	1.00	
5	СВ	MET	Α	16	64.933	50.049	-8.267	1.00	
8	CG	MET	Α	16	65.153	50.446	-9.726	1.00	47.01
11	SD	MET	Α	16	66.181	49.252	-10.631	1.00	50.95
12	CE	MET	Α	16	64.933	48.059	-11.220	1.00	50.52
16	С	MET	Α	16	63.907	52.030	-7.120	1.00	43.94
17	0	MET	Α	16	63.880	53.159	-7.610	1.00	44.23
20	N	ASP	Α	17	62.875	51.491	-6.466	1.00	42.41
22	CA	ASP	Α	17	61.591	52.188	-6.366	1.00	41.35
24	CB	ASP	Α	17	60.409	51.226	-6.459	1.00	41.74
27	CG		Α	17	59.134	51.926	-6.899	1.00	43.33
28	OD1	ASP		17	58.448	52.535	-6.037	1.00	46.33
29	OD2	ASP	A	17	58.753	51.939	-8.093	1.00	45.52
30	С		Α	17	61.486	52.990	-5.079	1.00	39.80
31	0	ASP	Α	17	61.195	52.441	-4.005	1.00	38.54
32	N	PHE	Α	18	61.672	54.298	-5.210	1.00	38.05
34	CA	PHE		18	61.858	55.146	-4.050	1.00	36.90
36	CB	PHE		18	62.429	56.514	-4.427	1.00	36.92
39	CG		Α	18	63.016	57.233	-3.260	1.00	36.41
40	CD1		A	18	64.116	56.707	-2.609	1.00	37.05
42	CE1	PHE	A	18	64.658	57.340	-1.502	1.00	36.55
44	CZ		A	18	64.098	58.493	-1.036	1.00	36.07
46	CE2	PHE	A	18	62.988	59.025	-1.664	1.00	36.56
48	CD2	PHE		18	62.442	58.392	-2.768	1.00	36.65
50	С	PHE		18	60.632	55.314	-3.158	1.00	35.80
51	0	PHE		18	60.769	55.198	-1.949	1.00	35.17
52	N	PRO		19	59.456	55.618	-3.712	1.00	34.90
53	CA	PRO		19	58.239	55.676	-2.889	1.00	34.06
55	CB	PRO		19	57.123	55.861	-3.924	1.00	34.29
58	CG CD	PRO		19	57.782	56.558	-5.047	1.00	34.27
61 64	CD	PRO		19	59.176	55.993	-5.114	1.00	34.77
65	0	PRO PRO	A	19 19	58.008	54.418	-2.039	1.00	33.38
66	N	GLN		20	57.585	54.564	-0.895	1.00	32.65
68	CA	GLN		20	58.279	53.228	-2.579	1.00	32.48
70	CB	GLN		20	58.126 58.188	51.981 50.746	-1.815	1.00	32.23
73	CG	GLN		20	56.883	50.746	-2.732 -3.534	1.00	32.68 35.01
76	CD	GLN		20	56.611	49.011	-3.534	1.00	39.06
77	OE1	GLN		20	55.463	48.546	-3.685	1.00	41.57
78	NE2	GLN		20	57.654	48.270	-4.193	1.00	39.95
81	C	GLN		20	59.177	51.869	-0.700	1.00	30.90
82	0	GLN		20	58.892	51.363	0.379	1.00	30.03
				-	-			• •	

FIGURE 3 (Cont.) AB

A	В	С	D	E		F	G	Н	I	J
83	N	GLN	Α	21	6	50.385	52.351	-0.959	1.00	29.82
85	CA	GLN	Α	21		51.426	52.370	0.058	1.00	29.68
87	CB	GLN	Α	21	6	52.783	52.738	-0.560	1.00	29.82
90	CG	GLN	Α	21	6	3.366	51.647	-1.494	1.00	31.98
93	CD	GLN	Α	21	6	3.920	50.425	-0.746	1.00	34.89
94	OE1	GLN	Α	21	6	4.483	49.512	-1.360	1.00	36.76
95	NE2	GLN	Α	21	6	3.762	50.412	0.572	1.00	37.29
98	C	GLN	Α	21	6	1.065	53.323	1.204	1.00	28.61
99	0	GLN	Α	21	6	51.214	52.973	2.372	1.00	28.03
100	N	LEU	Α	22	6	50.588	54.513	0.863	1.00	27.80
102	CA	LEU	Α	22	6	50.120	55.472	1.848	1.00	27.76
104	CB	LEU	Α	22	5	9.582	56.740	1.169	1.00	28.15
107	CG	LEU	Α	22	6	50.595	57.714	0.543	1.00	29.56
109	CD1	LEU	Α	22	9	9.880	58.764	-0.297	1.00	30.48
113	CD2	LEU	Α	22	6	51.447	58.392	1.611	1.00	30.42
117	С	LEU	Α	22	9	9.036	54.861	2.736	1.00	27.31
118	0	LEU	Α	22	9	9.099	54.975	3.950	1.00	26.43
119	N	GLU	Α	23	5	8.057	54.185	2.145	1.00	27.14
121	CA	GLU	Α	23	5	6.973	53.627	2.952	1.00	27.44
123	CB	GLU		23	5	55.760	53.232	2.101	1.00	28.34
126	CG	GLU	Α	23	9	4.798	52.234	2.759	1.00	31.44
129	CD	GLU	Α	23	5	3.961	52.789	3.912	1.00	35.82
130	OE1	GLU		23	5	2.791	52.370	4.024	1.00	38.87
131	OE2	GLU		23	5	4.448	53.597	4.738	1.00	38.87
132	C	GLU		23	5	7.465	52.462	3.805	1.00	26.15
133	0	GLU		23	5	7.040	52.322	4.949	1.00	25.29
134	N	ALA		24	9	8.357	51.642	3.254	1.00	25.31
136	CA	ALA		24		9.018	50.578	4.013	1.00	24.72
138	CB	ALA		24		0.019	49.847	3.153	1.00	25.46
142	С	ALA		24		9.728	51.160	5.230	1.00	24.33
143	0	ALA		24		9.610	50.636	6.331	1.00	23.33
144	N		Α	25		0.438	52.263	5.025	1.00	23.38
146	CA	CYS		25		51.130	52.944	6.115		23.00
148	CB	CYS		25		2.029	54.056	5.578		23.11
151	SG	CYS		25		2.861	54.980	6.885		21.11
152	C		Α	25		0.147	53.499	7.162	1.00	22.39
153	0	CYS		25		0.368	53.344	8.351	1.00	22.44
154	N	VAL		26		9.051	54.105	6.725		22.24
156	CA	VAL		26		8.056	54.638	7.651	1.00	
158	CB	VAL		26		6.889	55.349	6.902	1.00	
160	CG1	VAL		26		5.697	55.610	7.815		22.85
164	CG2	VAL		26		7.368	56.650	6.293		22.19
168	C	VAL		26		7.534	53.530	8.580		21.91
169	0	VAL		26		7.440	53.722	9.789		21.65
170	N	LYS		27		7.235	52.369	8.011		21.41
172	CA	LYS		27		6.741	51.236	8.779		21.24
174	CB	LYS		27		6.273	50.127	7.836		22.15
177	CG	LYS		27		4.982	50.454	7.081		24.03
180	CD	LYS		27		4.467	49.210	6.340	1.00	
183	CE	LYS		27		3.133	49.458	5.596	1.00	31.91
186	NZ	LYS		27		3.166	48.924	4.184		33.67
190	С	LYS	A	27	=	7.798	50.693	9.737	1.00	20.33

FIGURE 3 (Cont.)AC

Α	В	С	D	E	F	G	H	I	J
191	0	LYS		27	57.4			1.00	19.84
192	N	GLN		28	59.0			1.00	19.37
194	CA	GLN		28	60.1			1.00	19.22
196	CB	GLN		28	61.4			1.00	19.05
199	CG	GLN		28	62.5				19.21
202	CD	GLN		28	62.4			1.00	20.65
203	OE1	GLN		28	63.0				22.34
204	NE2	GLN		28	61.7			1.00	16.09
207	С	GLN		28	60.3				18.67
208	0	GLN		28	60.3				18.19
209	N	ALA		29	60.4				18.55
211	CA	ALA		29	60.74				18.70
213	CB	ALA		29	61.0			1.00	18.98
217	С	ALA		29	59.63				19.64
218 219	O N	ALA		29	59.8				19.64
221	N CA	ASN ASN		30 30	58.3				19.52
223					57.2			1.00	19.96
226	CB CG	ASN ASN		30 30	55.9			1.00	19.83
227	OD1	ASN		30	55.69 56.33			1.00	22.13
228	ND2	ASN		30	54.6				23.82
231	C	ASN		30	54.0			1.00	23.36 19.86
232	0	ASN		30	56.8			1.00	19.83
233	N	GLN		31	57.4				20.51
235	CA	GLN		31	57.5				21.34
237	СВ	GLN		31	57.9			1.00	
240	CG	GLN		31	57.8			1.00	
243	CD	GLN		31	58.0			1.00	
244	OE1	GLN		31	59.1			1.00	33.06
245	NE2	GLN		31	56.9			1.00	31.52
248	C	GLN		31	58.6			1.00	21.05
249	Ō	GLN		31	58.4				20.55
250	N	ALA		32	59.8			1.00	20.90
252	CA	ALA		32	60.9			1.00	21.59
254	CB	ALA		32	62.13				21.36
258	С	ALA		32	60.5				21.65
259	0	ALA	Α	32	60.6			1.00	
260	N	LEU	Α	33	59.9				22.61
262	CA	LEU		33	59.5				23.19
264	CB	LEU		33	58.93				23.47
267	CG	LEU	Α	33	59.8	79 55.966			24.21
269	CD1	LEU	Α	33	59.1			1.00	24.68
273	CD2	LEU	Α	33	60.39	91 56.88			26.09
277	С	LEU	Α	33	58.5	55 53.183	18.890	1.00	24.35
278	0	LEU	Α	33	58.6	59 53.39	L 20.094	1.00	23.66
279	N	SER	Α	34	57.50	57 52.47	l 18.356	1.00	25.27
281	CA	SER	Α	34	56.5	13 51.879	9 19.172	1.00	26.76
283	CB	SER	Α	34	55.4	30 51.162		1.00	27.01
286	OG	SER		34	54.78	39 52.07	7 17.470	1.00	28.06
288	С	SER		34	57.0				27.73
289	0	SER		34	56.5			1.00	28.77
290	N	ARG	Α	35	58.0	71 50.11	7 19.802	1.00	28.38

FIGURE 3 (Cont.)AD

A	В	С	D	E	F	G	Н	I	J
292	CA	ARG	Α	35	58.649	49.117	20.688	1.00	29.15
294	CB	ARG	A	35	59.580	48.182	19.915	1.00	29.68
297	CG	ARG	Α	35	58.842	47.176	19.053	1.00	33.37
300	CD	ARG	A	35	59.681	46.648	17.895	1.00	36.27
303	NE	ARG	Α	35	59.113	45.445	17.291	1.00	39.06
305	CZ	ARG	Α	35	59.778	44.630	16.473	1.00	41.04
306	NH1	ARG	Α	35	61.046	44.878	16.153	1.00	42.52
309	NH2	ARG	Α	35	59.174	43.564	15.970	1.00	42.39
312	С	ARG	Α	35	59.426	49.761	21.828	1.00	28.40
313	0	ARG	Α	35	59.480	49.210	22.926	1.00	27.74
314	N	PHE	Α	36	60.045	50.910	21.557	1.00	27.61
316	CA	PHE	Α	36	60.785	51.634	22.587	1.00	27.39
318	CB	PHE	Α	36	61.853	52.533	21.960	1.00	27.18
321	CG	PHE	Α	36	62.924	51.766	21.240		25.69
322	CD1	PHE		36	63.214	52.029	19.918	1.00	25.01
324	CE1	PHE	Α	36	64.194	51.311	19.253		25.43
326	CZ	PHE	Α	36	64.881	50.295	19.910	1.00	26.41
328	CE2		Α	36	64.600	50.022	21.218	1.00	26.08
330	CD2		Α	36	63.624	50.755	21.886	1.00	25.98
332	С	PHE		36	59.855	52.427	23.491	1.00	27.72
333	0	PHE		36	60.189	52.684	24.642	1.00	27.44
334	N	ILE		37	58.679	52.775	22.979	1.00	27.76
336	CA	ILE		37	57.677	53.488	23.756	1.00	28.44
338	CB	ILE	Α΄	37	56.779	54.342	22.815	1.00	28.50
340	CG1	ILE	Α	37	57.527	55.620	22.419	1.00	28.68
343	CD1	ILE	Α	37	56.932	56.377	21.266	1.00	29.67
347	CG2	ILE	Α	37	55.440	54.687	23.473	1.00	29.47
351	С	ILE		37	56.831	52.526	24.620	1.00	28.85
352	0	ILE		37	56.394	52.900	25.707	1.00	29.06
353	N	ALA		38	56.631	51.293	24.156	1.00	29.01
355	CA	ALA		38	55.688	50.357	24.797	1.00	29.51
357	CB	ALA		38	55.489	49.108	23.926	1.00	
361	C	ALA		38	55.995	49.951	26.251		29.76
362	0	ALA		38	55.058	49.805	27.032	1.00	30.41
363	N	PRO		39	57.261	49.761	26.631	1.00	
364	CA	PRO		39	57.590	49.430	28.028		29.81
366	CB	PRO		39	59.019	48.871	27.952		29.63
369	CG	PRO		39	59.465	48.986	26.511		30.25
372	CD	PRO		39		49.813			30.23
375 376	C 0	PRO		39	57.547	50.605	29.003		29.35
377	N	PRO LEU		39 40	57.768	50.409	30.200		29.40
379	CA	LEU		40	57.288 57.243	51.808 52.978	28.508		28.66
381	CB	LEU		40	57.243	54.260	29.364 28.535		27.78 27.92
384	CG	LEU		40	58.410	54.574	27.654		28.42
386		LEU		40	58.185	55.906			29.06
390	CD2	LEU		40	59.716	54.573			28.93
394	C	LEU		40	56.009		30.243		27.39
395	0	LEU		40		52.410	29.814		27.10
396	N	PRO		41		53.412	31.471		26.65
397	CA	PRO		41		53.506			26.24
399	СВ	PRO		41	55.528	53.818	33.719		26.42
				_					

FIGURE 3 (Cont.) AE

A	В	С	D	E	F	G	Н	I	J
402	CG	PRO	Α	41	56.887	54.444	33.440	1.00	26.56
405	CD	PRO	Α	41	57.339	53.909	32.122		26.41
408	С	PRO		41	54.017	54.624	31.863	1.00	25.76
409	0	PRO	Α	41	54.386	55.397	30.977	1.00	25.20
410	N	PHE	Α	42	52.840	54.706	32.469	1.00	25.70
412	CA	PHE		42	51.873	55.765	32.212	1.00	25.79
414	CB	PHE		42	52.479	57.131	32.556	1.00	25.87
417	CG	PHE		42	53.188	57.147	33.878	1.00	25.55
418	CD1		Α	42	52.489	56.876	35.049	1.00	
420	CE1		Α	42	53.131	56.864	36.274	1.00	25.51
422	CZ	PHE	Α	42	54.480	57.116	36.349	1.00	25.34
424	CE2		Α	42	55.195	57.379	35.186	1.00	25.76
426	CD2	PHE	Α	42	54.551	57.383	33.959	1.00	24.78
428	С	PHE		42	51.323	55.730	30.787	1.00	25.98
429	0	PHE	Α	42	50.987	56.762	30.226	1.00	25.18
430	N	GLN		43	51.222	54.528	30.221	1.00	26.46
432	CA	GLN	Α	43	50.537	54.330	28.942	1.00	27.47
434	CB	GLN	Α	43	50.502	52.854	28.527	1.00	27.56
437	CG	GLN	Α	43	51.828	52.229	28.185	1.00	28.72
440	CD	GLN	Α	43	52.596	52.968	27.106	1.00	30.09
441	OE1	GLN	Α	43	53.817	53.065	27.187	1.00	32.82
442	NE2	GLN	Α	43	51.897	53.475	26.096	1.00	30.99
445	С	GLN	Α	43	49.111	54.786	29.106	1.00	28.28
446	0	GLN	Α	43	48.511	54.598	30.172	1.00	28.52
447	N	ASN	Α	44	48.579	55.403	28.060	1.00	28.97
449	CA	ASN	A	44	47.202	55.868	28.040	1.00	29.76
451	CB	ASN	Α	44	46.212	54.687	28.180	1.00	30.31
454	CG	ASN		44	46.513	53.535	27.210	1.00	31.66
455	OD1	ASN	Α	44	46.576	53.726	25.997	1.00	36.40
456	ND2	ASN		44	46.694	52.342	27.748	1.00	32.76
459	С	ASN		44	46.937	56.948	29.094	1.00	29.56
460	0	ASN		44	45.842	57.041	29.631	1.00	29.84
461	N	THR		45	47.958	57.750	29.393	1.00	29.02
463	CA	THR		45	47.782	59.023	30.090	1.00	28.55
465	CB	THR		45	48.663	59.090	31.346	1.00	28.99
467	OG1	THR		45	50.045	59.094	30.966	1.00	29.70
469	CG2	THR		45	48.504	57.836	32.213	1.00	29.52
473	C	THR		45	48.173	60.135	29.107		27.72
474	0	THR		45	48.886	59.861	28.147		27.59
475	N	PRO		46	47.713	61.371	29.316		26.46
476	CA	PRO		46	47.961	62.453	28.351		25.93
478	CB	PRO		46	47.404	63.699	29.061		25.92
481	CG	PRO		46	46.331	63.155	29.974		26.20
484 487	CD C	PRO		46	46.879	61.831	30.447		26.74
488	0	PRO PRO		46 46	49.419	62.688 62.912	27.918 26.731		25.28 24.82
489	N	VAL		47	49.638 50.389	62.661	28.824		24.82
491	CA	VAL		47	51.766	62.944	28.412		24.49
493	СВ	VAL		47	52.711	63.189	29.616		24.35
495	CG1	VAL		47	52.934	61.920	30.414	1.00	
499	CG2	VAL		47	54.047	63.752	29.131		25.13
503	С	VAL		47	52.317	61.860	27.460		23.84

FIGURE 3 (Cont.) AF

Α	В	С	D	E	F	,	G	H	I	J
504	0	VAL		47	52.9		2.172	26.462		23.42
505	N	VAL		48	52.0		0.594	27.752		23.38
507	CA	VAL		48	52.5		9.516	26.878		23.48
509	CB	VAL		48	52.4		8.146	27.567		23.07
511	CG1	VAL		48	52.7		7.012	26.566		23.03
515	CG2	VAL		48	53.4		8.125	28.740	1.00	
519	С	VAL		48	51.7		9.512	25.567	1.00	
520	0	VAL		48	52.2		9.299	24.510		23.73
521	N	GLU		49	50.4		9.782	25.632		23.99
523	CA	GLU		49	49.6		9.897	24.417		24.17
525	CB	GLU		49	48.1		0.087	24.761		24.86
528	CG	GLU		49	47.5		8.863	25.404		27.67
531	CD	GLU		49	46.1		9.115	25.899		33.01
532	OE1	GLU		49	45.3		8.140	25.909		36.58
533	OE2	GLU		49	45.8		0.274	26.278	1.00	
534	С	GLU		49	50.1		1.066	23.562	1.00	22.99
535	0	GLU		49	50.0		0.980	22.345	1.00	21.91
536	N	THR		50	50.5	74 6	2.139	24.208	1.00	22.14
538	CA	THR		50	51.1	.47 6	3.270	23.497	1.00	21.71
540	CB	THR		50	51.4	26 6	4.447	24.442	1.00	21.87
542	OG1	THR		50	50.2	18 6	4.833	25.112		21.63
544	CG2	THR	Α	50	51.8	61 6	5.695	23.647	1.00	21.55
548	С	THR	Α	50	52.4	35 6	2.833	22.813	1.00	21.19
549	0	THR	Α	50	52.6	58 6	3.152	21.667	1.00	20.77
550	N	MET	Α	51	53.2	68 6	2.075	23.515	1.00	21.45
552	CA	MET	A	51	54.5	25 6	1.583	22.936	1.00	21.16
554	CB	MET	Α	51	55.3	21 6	0.768	23.965	1.00	21.28
557	CG	MET	Α	51	55.8	25 6	1.558	25.165	1.00	21.06
560	SD	MET	Α	51	56.5	03 6	0.485	26.448	1.00	21.92
561	CE	MET	Α	51	58.0	36 5	9.941	25.581	1.00	18.94
565	С		Α	51	54.2	27 6	0.713	21.704	1.00	21.05
566	0	MET	Α	51	54.8	73 6	0.858	20.676	1.00	21.01
567	N	GLN		52	53.2	28 5	9.835	21.812	1.00	21.04
569	CA	GLN		52	. 52 . 8	82 5	8.908	20.737	1.00	21.29
571	CB	GLN		52	51.8	62 5	7.889	21.229	1.00	21.77
574	CG	GLN		52	52.4		6.822	22.155	1.00	
577	CD	GLN	Α	52	51.2	97 5	5.954	22.728	1.00	26.61
578		GLN		52	51.2		4.743	22.480		30.25
579	NE2	GLN		52	50.3		6.569	23.474		24.83
582	С	GLN		52	52.2		9.642	19.526		21.06
583	0	GLN		52	52.5		9.291	18.371		19.85
584	N	TYR		53	51.4		0.656	19.804		20.82
586	CA	TYR		53	50.8		1.466	18.760		21.28
588	CB	TYR		53	49.9		2.447	19.433		21.43
591	CG	TYR		53	49.1		3.357	18.555		23.00
592	CD1	TYR		53	47.8		3.002	18.154		24.56
594	CE1	TYR		53	47.0		3.859	17.385		24.49
596	CZ	TYR		53	47.5		5.107	17.052		25.48
597	OH	TYR		53	46.7		5.965	16.292		24.53
599	CE2	TYR		53	48.8		5.484	17.445		23.07
601	CD2	TYR		53	49.6		4.618	18.212		23.55
603	С	TYR	A	53	51.9	67 6	2.218	18.002	1.00	20.79

FIGURE 3 (Cont.)AG

A	В	С	D	E	F		G	F	I	I	J
604	0	TYR	Α	53	52.033	62	.184	16.	765	1.00	20.35
605	N	GLY		54	52.811		.910		761	1.00	20.69
607	CA	GLY		54	53.840		.751		187	1.00	20.90
610	С	GLY		54	54.963		.972		526	1.00	21.30
611	0	GLY	Α	54	55.596	63	.495		627	1.00	21.54
612	N	ALA	Α	55	55.215	61	.732	17.	955	1.00	21.95
614	CA	ALA	Α	55	56.315		.942		389	1.00	22.16
616	CB	ALA	Α	55	56.981	60	.100	18.	480	1.00	22.04
620	С	ALA	Α	55	55.862	60	.033	16.	242	1.00	22.84
621	0	ALA	Α	55	56.609	59	.808	15.	282	1.00	22.77
622	N	LEU	Α	56	54.645	59	.506	16.	337	1.00	23.82
624	CA	LEU	Α	56	54.227	58	.413	15.	446	1.00	25.01
626	CB	LEU	Α	56	53.718	57	.229	16.	272	1.00	25.40
629	CG	LEU	Α	56	54.803	56	.448	16.	999	1.00	26.02
631	CD1	LEU	Α	56	54.192	55	.617	18.	110	1.00	27.58
635	CD2	LEU	Α	56	55.583	55	.570	16.	011	1.00	26.63
639	C	LEU	Α	56	53.188	58	.758	14.	386	1.00	25.71
640	0	LEU	Α	56	53.144	58	.088	13.	352	1.00	25.79
641	N	LEU	Α	57	52.351	59	.772	14.	626	1.00	26.23
643	CA	LEU	Α	57	51.244	60	.076	13.	712	1.00	26.84
645	CB	LEU	Α	57	50.045	60	.627	14.	487	1.00	27.25
648	CG	LEU	Α	57	48.675	60	.380	13.	836	1.00	29.61
650	CD1	LEU	Α	57	48.417	58	.886	13.	617	1.00	30.97
654	CD2	LEU	Α	57	47.544	60	.990	14.	672	1.00	31.15
658	С	LEU	Α	57	51.660	61	.041	12.	589	1.00	26.56
659	0	LEU	Α	57	51.650	62	.260	12.	762	1.00	26.92
660	N	GLY	Α	58	52.014	60	.471	11.	441	1.00	26.04
662	CA	GLY	Α	58	52.480	61	230	10.	294	1.00	25.24
665	C	GLY	Α	58	53.983		.421	10.	347	1.00	24.44
666	0	GLY		58	54.635	61	.015		301	1.00	24.64
667	N	GLY		59	54.513	62	.081	9.	331	1.00	23.73
669	CA	GLY		59	55.938		.322		195	1.00	23.06
672	C	GLY		59	56.553		359		209	1.00	22.26
673	0	GLY		59	56.162		.194	8 .	133	1.00	22.42
674	N	LYS		60	57.547		.842	7.	478	1.00	22.13
676	CA		Α	60	58.154		.112		374	1.00	21.99
678	CB	LYS		60	58.759		.101		373	1.00	22.38
681	CG	LYS		60	57.740		.053		741		22.42
684	CD	LYS		60	58.397		.946		700	1.00	22.36
687	CE	LYS		60	59.309		.000		315	1.00	22.65
690	NZ	LYS		60	58.610		.764		390	1.00	22.32
694	C	LYS		60	59.236		.121		820	1.00	21.22
695	0	LYS		60	59.639		.250		044	1.00	21.45
696	N	ARG		61	59.679		.268		064	1.00	20.48
698	CA	ARG		61	60.763		.494		657	1.00	19.82
700	CB	ARG		61	60.347		.035		877	1.00	19.66
703	CG	ARG		61	59.138		.855		723	1.00	20.10
706	CD	ARG		61	59.272		.230		192	1.00	20.40
709	NE CZ	ARG		61	57.948		.049		781	1.00	20.92
711	CZ	ARG		61	57.037		.991		934	1.00	22.13
712	NH1	ARG		61	57.298		.255		645	1.00	23.06
715	NH2	ARG	А	61	55.840	58	.667	12.	421	1.00	22.86

FIGURE 3 (Cont.) AH

Α	В	C	D	E	F	G	H	I	J
	_		_						
718	C	ARG		61	62.061	59.514	7.860	1.00	19.24
719	0	ARG		61	62.738	58.501	7.779	1.00	18.48
720	N	LEU		62	62.432	60.666	7.307	1.00	18.87
722	CA	LEU		62	63.630	60.734	6.485	1.00	18.40
724	CB	LEU		62	63.643	61.988	5.629	1.00	18.86
727	CG	LEU		62	62.430	62.083	4.708	1.00	18.30
729	CD1	LEU		62	62.550	63.320	3.821	1.00	18.04
733	CD2	LEU		62	62.266	60.815	3.896	1.00	19.13
737	C	LEU		62	64.908	60.646	7.296	1.00	18.46
738	0	LEU		62	65.933	60.241	6.772	1.00	18.88
739	N	ARG		63	64.866	61.017	8.562	1.00	17.65
741	CA	ARG		63	66.054	60.871	9.384	1.00	17.87
743	CB	ARG		63	66.000	61.756	10.611	1.00	17.85
746	CG	ARG		63	66.045	63.219	10.223	1.00	17.38
749	CD	ARG		63	65.459	64.177	11.253	1.00	17.84
752	NE	ARG		63	65.361	65.533	10.704	1.00	19.01
754	CZ	ARG		63	64.417	65.941	9.863	1.00	20.05
755	NH1	ARG		63	64.422	67.193	9.411	1.00	22.90
758	NH2	ARG		63	63.449	65.123	9.477	1.00	21.09
761	С	ARG		63	66.322	59.401	9.705	1.00	17.71
762	0	ARG		63	67.454	58.951	9.531	1.00	18.10
763	N	PRO		64	65.329	58.645	10.163	1.00	17.51
764	CA	PRO		64	65.476	57.180	10.192	1.00	17.45
766	CB	PRO		64	64.070	56.703	10.531	1.00	17.56
769	CG	PRO	Α	64	63.506	57.791	11.356	1.00	17.73
772	CD	PRO	Α	64	64.052	59.064	10.767	1.00	17.18
775	С	PRO	Α	64	65.936	56.615	8.859	1.00	17.33
776	0	PRO	Α	64	66.816	55.755	8.854	1.00	17.25
777	N	PHE	Α	65	65.376	57.104	7.754	1.00	17.93
779	CA	PHE	Α	65	65.781	56.677	6.427	1.00	18.40
781	CB	PHE	Α	65	65.044	57.457	5.338	1.00	19.10
784	CG	PHE	À	65	65.198	56.872	3.941	1.00	19.82
785	CD1	PHE	Α	65	66.425	56.898	3.278	1.00	21.48
787	CE1	PHE	Α	65	66.558	56.356	1.990	1.00	24.16
789	CZ	PHE	Α	65	65.456	55.801	1.354	1.00	23.70
791	CE2	PHE	Α	65	64.232	55.787	2.000	1.00	24.40
793	CD2	PHE	Α	65	64.112	56.329	3.289	1.00	21.85
795	С	PHE	Α	65	67.288	56.831	6.274	1.00	18.39
796	0	PHE	Α	65	67.951	55.920	5.814	1.00	18.40
797	N	LEU	Α	66	67.820	57.973	6.683	1.00	18.52
799	CA	LEU	Α	66	69.255	58.228	6.643	1.00	18.77
801	CB	LEU	Α	66	69.554	59.650	7.101	1.00	19.16
804	CG	LEU	Α	66	69.280	60.737	6.070	1.00	20.56
806	CD1	LEU	Α	66	69.409	62.108	6.739	1.00	21.70
810	CD2	LEU	Α	66	70.233	60.611	4.897	1.00	21.14
814	С	LEU	Α	66	70.063	57.274	7.512	1.00	18.22
815	0	LEU		66	71.162	56.862	7.131	1.00	17.84
816	N	VAL		67	69.546	56.973	8.693	1.00	16.88
818	CA	VAL	Α	67	70.235	56.066	9.609	1.00	17.06
820	CB	VAL		67	69.512	56.001	10.969	1.00	16.98
822	CG1	VAL		67	70.075	54.909	11.865	1.00	17.14
826	CG2	VAL	A	67	69.621	57.337	11.679	1.00	16.69

FIGURE 3 (Cont.) AI

A	В	С	D	E	F	G	Н	I	J
830	С	VAL	Α	67	70.315	54.667	8.984	1.00	17.43
831	0	VAL	Α	67	71.391	54.087	8.924	1.00	16.85
832	N	TYR	Α	68	69.171	54.175	8.504	1.00	17.82
834	CA	TYR	Α	68	69.049	52.853	7.890	1.00	18.73
836	CB	TYR	Α	68	67.590	52.546	7.534	1.00	18.65
839	CG	TYR	Α	68	66.682	52.294	8.706	1.00	17.77
840	CD1	TYR	Α	68	66.993	51.343	9.670	1.00	18.53
842	CE1	TYR	Α	68	66.152	51.109	10.734	1.00	19.24
844	CZ	TYR	Α	68	64.967	51.819	10.844	1.00	17.86
845	OH	TYR	Α	68	64.123	51.616	11.915	1.00	16.87
847	CE2	TYR	Α	68	64.650	52.774	9.914	1.00	18.34
849	CD2	TYR	Α	68	65.492	52.988	8.835	1.00	18.14
851	С	TYR	Α	68	69.878	52.741	6.626	1.00	19.22
852	0	TYR	Α	68	70.627	51.788	6.466	1.00	20.65
853	N	ALA	Α	69	69.762	53.725	5.744	1.00	19.41
855	CA	ALA	Α	69	70.470	53.707	4.474	1.00	19.53
857	CB	ALA	Α	69	70.035	54.875	3.616	1.00	20.02
861	С	ALA	Α	69	71.975	53.744	4.695	1.00	20.18
862	0	ALA	Α	69	72.721	53.053	4.011	1.00	21.39
863	N	THR	Α	70	72.423	54.545	5.656	1.00	20.00
865	CA	THR	Α	70	73.841	54.656	5.930	1.00	20.26
867	СВ	THR	Α	70	74.124	55.842	6.828	1.00	20.06
869	OG1	THR	Α	70	73.742	57.060	6.143	1.00	19.95
871	CG2	THR	Α	70	75.624	55.979	7.077	1.00	20.73
875	С	THR	Α	70	74.371	53.370	6.527	1.00	20.27
876	0	THR	Α	70	75.330	52.821	6.025	1.00	20.97
877	N	GLY	Α	71	73.743	52.886	7.588	1.00	20.36
879	CA	GLY	Α	71	74.136	51.630	8.199	1.00	20.44
882	C	GLY	Α	71	74.090	50.470	7.229	1.00	20.43
883	0	GLY	Α	71	74.966	49.600	7.242	1.00	21.38
884	N	HIS	Α	72	73.061	50.442	6.393	1.00	21.26
886	CA	HIS	Α	72	72.886	49.367	5.401	1.00	21.95
888	CB	HIS	Α	72	71.577	49.530	4.623	1.00	22.16
891	CG	HIS	Α	72	70.369	49.049	5.362	1.00	21.95
892	ND1	HIS	Α	72	69.094	49.468	5.051	1.00	23.29
894	CE1	HIS	Α	72	68.231	48.892	5.869	1.00	23.63
896	NE2	HIS	Α	72	68.899	48.097	6.687	1.00	21.16
898	CD2	HIS	Α	72	70.238	48.181	6.394	1.00	22.72
900	С	HIS	Α	72	74.054	49.313	4.421	1.00	22.56
901	0	HIS	Α	72	74.455	48.228	3.995	1.00	21.64
902	N	MET	Α	73	74.610	50.477	4.080	1.00	23.05
904	CA	MET	Α	73	75.782	50.536	3.201	1.00	23.89
906	CB	MET	Α	73	76.282	51.961	3.027	1.00	24.12
909	CG	MET	Α	73	75.546	52.765	2.016	1.00	26.38
912	SD	MET	Α	73	76.590	54.090	1.347	1.00	31.06
913	CE	MET	A	73	77.179	54.849	2.837	1.00	30.61
917	С	MET	A	73	76.944	49.713	3.732	1.00	24.04
918	0	MET	Α	73	77.740	49.208	2.945	1.00	24.70
919	N	PHE	A	74	77.052	49.617	5.057	1.00	24.12
921	CA	PHE	Α	74	78.122	48.863	5.723	1.00	24.15
923	CB	PHE	Α	74	78.644	49.693	6.881	1.00	24.28
926	CG	PHE	Α	74	79.127	51.040	6.455	1.00	25.09

FIGURE 3 (Cont.)AJ

Α	В	C	D	E	F	G	Н	I	J
927	CD1	PHE	Α	74	78.410	52.183	6.759	1 00	25.88
929	CE1	PHE		74	78.847	53.424	6.357	1.00	25.67
931	CZ	PHE		74	80.015	53.424	5.641	1.00	26.11
933	CE2		A	74	80.751	52.415	5.330	1.00	26.51
935	CD2	PHE		74	80.305				
937	CDZ	PHE		74 74		51.167	5.736	1.00	26.10
				74 74	77.710	47.461	6.196	1.00	
938 939	O N		A N		78.475	46.770	6.875	1.00	
		GLY		75 75	76.508	47.039	5.815	1.00	23.45
941 944	CA C	GLY GLY		75 75	76.025	45.708	6.114		23.38
945	0	GLY		75 75	75.544	45.539 44.415	7.545		23.11
	N			75 76	75.412		8.032		22.14
946 948	CA	VAL VAL		76 76	75.261	46.636	8.241		22.50
950	CB	VAL			74.698	46.461	9.577	1.00	22.69
952	CG1	VAL		76 76	75.093	47.576	10.642	1.00	22.92
956	CG2	VAL		76 76	75.915 73.908	48.711 48.074	10.067	1.00	23.76
960	C	VAL		76 76	73.306		11.396	1.00	22.71
961	0	VAL		76 76		46.144	9.484	1.00	
962	N	SER		70 77	72.487 72.746	46.604 45.302	8.591 10.402	1.00	21.42 21.48
964	CA	SER		77	71.389	44.778	10.402		21.46
966	CB	SER		77	71.250	43.671	11.467		22.01
969	OG	SER		77	69.901	43.269	11.656	1.00	24.55
971	C	SER		77	70.388	45.893	10.669	1.00	21.66
972	0	SER		77	70.586	46.768	11.497	1.00	20.52
973	N	THR		78	69.280	45.849	9.950	1.00	21.30
975	CA	THR		78	68.197	46.782	10.145		21.37
977	CB	THR		78	67.041	46.395	9.243	1.00	
979	OG1	THR		78	67.522	46.238	7.898	1.00	
981	CG2	THR		78	66.004	47.531	9.175	1.00	21.88
985	C	THR		78	67.742	46.839	11.609		21.40
986	0	THR		78	67.457	47.919	12.127		20.26
987	N	ASN		79	67.712	45.681	12.273		20.85
989	CA	ASN		79	67.259	45.592	13.665		21.11
991	СВ	ASN		79	67.155	44.113	14.110	1.00	20.78
994	CG	ASN		79	66.777	43.962	15.577	1.00	20.57
995	OD1	ASN		79	65.629	44.176	15.960	1.00	20.74
996	ND2	ASN	Α	79	67.741	43.572	16.395		21.96
999	С	ASN	Α	79	68.135	46.366	14.648	1.00	21.18
1000	0	ASN	Α	79	67.630	46.935	15.589	1.00	21.24
1001	N	THR	Α	80	69.445	46.363	14.445	1.00	21.31
1003	CA	THR	Α	80	70.325	47.176	15.288	1.00	22.18
1005	CB	THR	Α	80	71.831	46.719	15.233	1.00	23.07
1007	OG1	THR	Α	80	72.729	47.845	15.254	1.00	25.14
1009	CG2	THR	Α	80	72.163	46.051	13.972	1.00	25.36
1013	C	THR		80	70.149	48.653	14.952		21.28
1014	0	THR	Α	80	70.191	49.488	15.836	1.00	21.18
1015	N	LEU		81	69.889	48.958	13.685	1.00	
1017	CA	LEU		81	69.699	50.338	13.267	1.00	19.67
1019	CB	LEU		81	69.773	50.458	11.743	1.00	19.03
1022	CG	LEU		81	71.174	50.220	11.203		20.05
1024	CD1	LEU		81	71.133	49.777	9.747		20.55
1028	CD2	LEU	Α	81	72.025	51.477	11.362	1.00	21.66

FIGURE 3 (Cont.) AK

Α	В	С	D	E	F	G	H	I	J
	_		_						
1032	C	LEU		81	68.395	50.943	13.785	1.00	19.10
1033	0	LEU		81	68.266	52.154	13.797	1.00	17.73
1034	N	ASP	A	82	67.452	50.098	14.213	1.00	18.92
1036	CA	ASP	A	82	66.206	50.555	14.808	1.00	19.26
1038	CB	ASP		82	65.374	49.380	15.347	1.00	19.80
1041	CG	ASP		82	64.537	48.689	14.279	1.00	21.07
1042	OD1	ASP	A	82	64.370	49.232	13.167	1.00	22.88
1043	OD2	ASP	A	82	63.977	47.584	14.496	1.00	22.05
1044	C	ASP		82	66.491	51.503	15.972	1.00	18.72
1045	0	ASP		82	65.743	52.455	16.193	1.00	18.90
1046	N	ALA		83	67.551	51.227	16.724	1.00	18.47
1048	CA	ALA		83	67.879	52.031	17.902	1.00	18.05
1050	CB C	ALA		83	68.957	51.350	18.777	1.00	18.08
1054		ALA		83	68.262	53.464	17.528	1.00	17.75
1055	O N	ALA		83	67.571	54.391	17.954	1.00	16.58
1056	N	PRO		84	69.334	53.674	16.754	1.00	17.46
1057 1059	CA CB	PRO PRO		84 84	69.660 70.978	55.034	16.310	1.00	17.24 17.48
1059	CG	PRO		84	71.073	54.870 53.397	15.537 15.176	1.00	17.40
1062	CD	PRO		84	70.318	52.690	16.274	1.00	17.39
1068	CD	PRO		84	68.570	55.674	15.452	1.00	17.54
1069	0	PRO		84	68.372	56.871	15.432	1.00	16.99
1070	N	ALA		85	67.881	54.899	14.617	1.00	17.55
1070	CA	ALA		85	66.786	55.439	13.827	1.00	17.51
1074	CB	ALA		85	66.196	54.371	12.908	1.00	17.15
1078	C	ALA		85	65.710	56.010	14.751	1.00	17.33
1079	ō	ALA		85	65.235	57.120	14.540	1.00	17.48
1080	N	ALA		86	65.365	55.276	15.797	1.00	17.28
1082	CA	ALA		86	64.309	55.702	16.702	1.00	17.98
1084	CB	ALA		86	63.858	54.558	17.575	1.00	17.95
1088	C	ALA		86	64.764	56.881	17.559	1.00	18.07
1089	Ō	ALA		86	63.986	57.800	17.828	1.00	18.55
1090	N	ALA		87	66.027	56.852	17.965	1.00	17.63
1092	CA	ALA		87	66.612	57.905	18.776	1.00	17.90
1094	CB	ALA		87	68.016	57.551	19.129	1.00	17.89
1098	С	ALA	Α	87	66.602	59.238	18.046	1.00	18.01
1099	0	ALA	Α	87	66.199	60.258	18.611	1.00	16.96
1100	N	VAL		88	67.076	59.233	16.802	1.00	18.36
1102	CA	VAL		88	67.108	60.469	16.022	1.00	
1104	CB	VAL	Α	88	67.919	60.359	14.706	1.00	
1106	CG1	VAL	Α	88	69.346	59.943	15.004	1.00	21.38
1110	CG2	VAL	Α	88	67.262	59.431	13.694	1.00	20.88
1114	С	VAL	Α	88	65.697	60.984	15.728	1.00	18.91
1115	0	VAL	Α	88	65.478	62.192	15.694	1.00	19.41
1116	N	GLU	Α	89	64.755	60.075	15.506	1.00	18.77
1118	CA	GLU	Α	89	63.371	60.460	15.281	1.00	19.03
1120	CB	GLU		89	62.580	59.307	14.672	1.00	19.35
1123	CG	GLU		89	61.202	59.659	14.140	1.00	
1126	CD	GLU		89	61.187	60.686	13.014		23.08
1127	OE1			89	60.085	61.188	12.699		21.79
1128		GLU		89	62.243	61.001	12.436		22.95
1129	С	GLU	Α	89	62.726	60.972	16.571	1.00	19.06

FIGURE 3 (Cont.) AL

Α	В	С	D	E	F	G	Н	I	J
	_		_						
1130	0	GLU		89	61.883	61.856	16.515	1.00	18.98
1131	N	CYS		90	63.154	60.466	17.724	1.00	19.07
1133	CA		A	90	62.684	61.026	18.999	1.00	19.48
1135	CB	CYS		90	63.154	60.218	20.204	1.00	19.62
1138	SG	CYS		90	62.240	58.692	20.462	1.00	
1139	C	CYS	A	90	63.139	62.464	19.144	1.00	18.83
1140	0	CYS	A	90	62.348	63.311	19.526	1.00	19.11
1141	N	ILE		91	64.405	62.740	18.846	1.00	18.13
1143	CA	ILE		91	64.900	64.108	18.934	1.00	17.94
1145	CB	ILE		91	66.402	64.201	18.602	1.00	18.00
1147	CG1	ILE		91	67.269	63.442	19.628	1.00	18.23
1150	CD1	ILE		91	67.160	63.942	21.057	1.00	18.91
1154	CG2	ILE		91	66.824	65.659	18.520	1.00	18.94
1158	C	ILE		91	64.117	64.994	17.959	1.00	17.15
1159	0	ILE		91	63.700	66.094	18.308	1.00	16.79
1160	N	HIS		92	63.952	64.506	16.732	1.00	16.32
1162	CA	HIS	A	92	63.238	65.238	15.701	1.00	16.58
1164	CB	HIS	A	92	63.182	64.438	14.409	1.00	16.65
1167	CG	HIS HIS	A.	92 92	62.424	65.119	13.321	1.00	16.27
1168					61.352	64.536	12.675	1.00	17.53
1170		HIS		92	60.892	65.378	11.761	1.00	15.88
1172			A A	92 92	61.620	66.480	11.800	1.00	17.29
1174					62.573	66.348	12.779	1.00	15.01
1176 1177	C 0	HIS HIS	A	92 92	61.825	65.555	16.167	1.00	16.53
					61.399	66.712	16.151	1.00	16.57
1178	N CA	ALA ALA		93 93	61.119	64.532	16.620	1.00	15.86
1180 1182	CB	ALA		93 93	59.753	64.699	17.119	1.00	16.23
1186	С	ALA		93	59.177 59.671	63.346	17.566	1.00	16.25
1187	0	ALA		93	58.753	65.720 66.544	18.251 18.297	1.00	16.36
1188	N	TYR		94	60.632	65.668	19.168	1.00	16.22 16.81
1190	CA	TYR		94	60.653	66.585	20.289	1.00	17.25
1192	CB	TYR		94	61.742	66.187	21.312	1.00	18.09
1195	CG	TYR		94	62.785	67.233	21.639	1.00	18.65
1196	CD1	TYR		94	62.444	68.391	22.309	1.00	20.51
1198	CE1	TYR		94	63.388	69.341	22.613	1.00	22.48
1200	CZ	TYR		94	64.701	69.138	22.248	1.00	
1201	ОН	TYR		94	65.628	70.083	22.565		24.51
1203	CE2			94	65.075	67.983	21.590	1.00	
1205	CD2	TYR		94	64.122	67.037	21.306	1.00	
1207	С	TYR		94	60.837	68.001	19.766	1.00	
1208	0	TYR		94	60.178	68.921	20.232		16.91
1209	N	SER		95	61.709	68.169	18.780		17.12
1211	CA	SER		95	62.028	69.486	18.281	1.00	
1213	CB	SER		95	63.209	69.446	17.312	1.00	
1216	OG	SER		95	62.859	68.946	16.045	1.00	
1218	C	SER		95	60.787	70.161	17.665	1.00	18.18
1219	0	SER		95	60.591	71.367	17.826	1.00	17.08
1220	N	LEU		96	59.936	69.376	17.021	1.00	18.08
1222	CA	LEU		96	58.748	69.937	16.356	1.00	18.75
1224	CB	LEU		96	58.168	68.946	15.359	1.00	18.81
1227	CG	LEU	Α	96	59.159	68.371	14.350	1.00	19.61

FIGURE 3 (Cont.) AM

A	В	С	D	E	F	G	Н	I	J
1229	CD1	LEU	Α	96	58.421	67.472	13.385	1.00	19.87
1233	CD2	LEU		96	59.901	69.477	13.628		20.82
1237	C	LEU		96	57.676	70.285	17.371		18.79
1238	ō	LEU		96	56.928	71.252	17.192	1.00	
1239	И	ILE		97	57.581	69.478	18.422	1.00	18.80
1241	CA	ILE		97	56.574	69.704	19.448	1.00	18.69
1243	CB	ILE		97	56.590	68.612	20.520	1.00	18.23
1245	CG1	ILE		97	56.062	67.307	19.941	1.00	17.66
1248	CD1	ILE		97	56.002	66.149	20.924	1.00	19.38
1252	CG2	ILE		97	55.756	69.050	21.746	1.00	18.51
1256	C	ILE		97	56.844	71.069	20.071	1.00	19.44
1257	0	ILE		97	55.925	71.851	20.071	1.00	19.44
1258	N	HIS		98	58.108	71.358	20.233		19.42
1260	CA	HIS		98	58.452	72.609	21.039		20.66
1262	CB	HIS		98	59.797	72.503	21.730		21.50
1265	CG	HIS		98	59.735	71.795	23.045		25.90
1266		HIS		98	59.610	70.432	23.149		34.19
1268		HIS	A	98	59.570	70.432	24.425		32.41
1270	NE2	HIS	A	98	59.660	71.175	25.149		32.34
1272		_	A	98	59.748	72.261	24.312		32.88
1274	C		A	98	58.437	73.774			
1275	0	HIS		98	58.095		20.072 20.444		20.22
1275	N	ASP		99	58.809	74.880 73.500			20.04
1278	CA	ASP		99	58.834		18.829		20.34
1280	CB	ASP		99	59.394	74.488 73:845	17.772 16.496		20.27 20.14
1283	CG		A	99	59.438	74.806	15.326		
1284		_	A	99	58.542	74.720	14.458	1.00	19.89 20.18
1285	OD2		A	99	60.332	75.665	15.194		18.02
1286	C	ASP	A	99	57.447	75.081	17.512		20.91
1287	0	ASP	A	99	57.322	76.277	17.253		21.26
1288	N	ASP		100	56.410	74.254	17.580		21.26
1290	CA	ASP		100	55.037	74.234	17.328		21.41
1292	СВ		A	100	54.098	73.551	17.328		21.41
1295	CG	ASP		100	54.436	72.819	15.799		20.29
1296		ASP		100	54.167	71.594	15.734		20.29
1297	OD2	ASP		100	54.978	73.379	14.841	1.00	
1298	C	ASP		100	54.428	75.500	18.483		21.71
1299	Ō	ASP		100	53.395	76.123	18.301		22.06
1300	N	LEU		101	55.039	75.467	19.664		21.73
1302	CA	LEU		101	54.463	76.129	20.837		21.71
1304	СВ	LEU		101	55.389	76.027	22.052		21.29
1307	CG	LEU		101	55.643	74.639	22.631		21.02
1309		LEU		101	56.681	74.748	23.744		21.63
1313		LEU		101	54.375	73.987	23.130		21.37
1317	C	LEU		101	54.173	77.611	20.587		22.13
1318	Ō	LEU		101	54.852	78.255	19.795		21.48
1319	N	PRO		102	53.167	78.152	21.273		23.19
1320	CA	PRO		102	52.850	79.588	21.175	1.00	
1322	СВ	PRO		102	51.811	79.779	22.282	1.00	
1325	CG	PRO		102	51.099	78.464	22.308	1.00	
1328	CD	PRO		102	52.216	77.443	22.149	1.00	
1331	С	PRO		102	54.045	80.533	21.348		24.21

FIGURE 3 (Cont.)AN

1332	Α	В	С	D	E	F	G	H	I	J
1333 N ALA A 103 54,943 80.255 22,285 1.00 24,74 1335 CA ALA A 103 56,123 81.094 22,516 1.00 25,23 1341 C ALA A 103 56,753 80.737 23,867 1.00 25,46 1342 O ALA A 103 58.093 81.742 21,417 1.00 25,46 1343 N MET A 104 57.981 79.590 19,550 1.00 26,00 1347 CB MET A 104 58.997 77.719 20,916 1.00 25.79 1350 CB MET A 104 58.997 77.719 20,916 1.00 25.79 1355 CB MET A 104 57.345 79.995 18.207 1.00 25.54 1356 CB MET A 104 57.345										
1335 CA ALA A 103 56.123 81.094 22.516 1.00 25.23 1337 CB ALA A 103 56.753 80.737 23.867 1.00 25.78 1341 C ALA A 103 58.093 81.742 21.317 1.00 24.70 1343 N MET A 104 57.053 79.879 20.626 1.00 25.19 1345 CA MET A 104 57.981 79.590 1.00 25.79 1350 CG MET A 104 58.362 78.109 19.598 1.00 25.79 1350 CG MET A 104 58.997 77.719 20.916 1.00 27.52 1353 SD MET A 104 57.345 79.995 18.207 1.00 25.73 1354 CE MET A 104 57.345 79.938 17.374 1.00 25.29 1356 O MET A 104 57.233 79.388 16.061 1.00 25.29		0								
1337 CB										
1341 C ALA A 103 57.176 80.941 21.417 1.00 25.46 1343 N MET A 104 57.053 79.879 20.626 1.00 25.70 1345 CA MET A 104 57.953 79.879 20.526 1.00 25.79 1350 CG MET A 104 58.997 77.719 20.916 1.00 25.79 1353 SD MET A 104 60.690 78.194 20.987 1.00 31.55 1354 CE MET A 104 61.411 77.093 19.688 1.00 31.55 1358 C MET A 104 57.213 81.186 17.942 1.00 25.54 1360 N ASP A 105 56.377 79.038 17.374 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.24 1369 OD2 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>1.00</td> <td>25.23</td>									1.00	25.23
1342 C ALA A 103 58.093 81.742 21.317 1.00 25.19 1345 CA MET A 104 57.081 79.590 19.550 1.00 25.19 1347 CB MET A 104 58.362 78.109 19.598 1.00 25.79 1350 CG MET A 104 58.997 77.719 20.916 1.00 27.52 1353 SD MET A 104 61.411 77.093 19.688 1.00 31.97 1358 C MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.345 79.938 17.374 1.00 25.24 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.28 1362 CA ASP A 105 56.832 78.419 14.969 1.00 25.24 1362 CG										
1343 N MET A 104 57.053 79.879 20.626 1.00 25.19 1347 CB MET A 104 57.981 79.590 19.550 1.00 26.00 1350 CG MET A 104 58.997 77.719 20.916 1.00 27.52 1353 SD MET A 104 60.690 78.194 20.987 1.00 31.55 1354 CE MET A 104 61.411 77.093 19.688 1.00 31.97 1358 C MET A 104 57.345 79.995 18.207 1.00 25.73 1360 N ASP A 105 56.373 79.388 16.061 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 24.83 1364 CB ASP A 105 58.853 77.642 13.954 1.00 22.92 1369 OD2 <td></td>										
1345 CA MET A 104 57.981 79.590 19.550 1.00 26.00 1347 CB MET A 104 58.362 78.109 19.598 1.00 25.79 1353 SD MET A 104 60.690 78.194 20.987 1.00 27.52 1354 CE MET A 104 61.411 77.093 19.688 1.00 31.97 1358 C MET A 104 57.345 79.995 18.207 1.00 25.73 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.54 1364 CB ASP A 105 56.837 79.038 16.061 1.00 25.24 1367 CG ASP A 105 56.873 79.388 16.061 1.00 25.24 1367 CG ASP A 105 58.853 77.642 13.954 1.00 26.02 1369 OD2 </td <td></td>										
1347 CB MET A 104 58.362 78.109 19.598 1.00 25.79 1353 SD MET A 104 58.997 77.719 20.916 1.00 27.52 1353 SD MET A 104 60.690 78.194 20.987 1.00 31.55 1354 CE MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.345 79.995 18.207 1.00 25.73 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.21 1367 CG ASP A 105 58.319 78.496 14.716 1.00 25.24 1367 CA ASP A 105 58.813 79.364 15.253 1.00 25.62 1370 C <td></td> <td></td> <td></td> <td></td> <td></td> <td>57.053</td> <td>79.879</td> <td>20.626</td> <td>1.00</td> <td>25.19</td>						57.053	79.879	20.626	1.00	25.19
1350 CG MET A 104 58.997 77.719 20.916 1.00 27.52 1353 SD MET A 104 60.690 78.194 20.987 1.00 31.55 1354 CE MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.213 81.186 17.942 1.00 25.54 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.29 1362 CA ASP A 105 56.837 79.038 16.061 1.00 25.24 1367 CG ASP A 105 56.873 79.038 16.061 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 22.09 1369 OD2 ASP A 105 54.851 <td></td>										
1353 SD MET A 104 60.690 78.194 20.987 1.00 31.55 1354 CE MET A 104 61.411 77.093 19.688 1.00 31.97 1358 C MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.213 81.186 17.942 1.00 25.54 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.29 1362 CA ASP A 105 56.832 78.419 14.969 1.00 25.24 1367 CG ASP A 105 58.853 77.642 13.954 1.00 22.99 1369 OD2 ASP A 105 54.851 79.525 16.069 1.00 26.92 1371 O ASP A 105 54.289				A		58.362		19.598	1.00	25.79
1354 CE MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.345 79.995 18.207 1.00 25.54 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.29 1362 CA ASP A 105 56.373 79.388 16.061 1.00 25.29 1367 CG ASP A 105 56.832 78.419 14.969 1.00 25.24 1367 CG ASP A 105 58.8319 78.496 14.716 1.00 22.09 1369 OD2 ASP A 105 54.851 79.525 16.069 1.00 25.92 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.289 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>1.00</td> <td>27.52</td>									1.00	27.52
1358 C MET A 104 57.345 79.995 18.207 1.00 25.73 1359 O MET A 104 57.213 81.186 17.942 1.00 25.54 1360 N ASP A 105 56.373 79.388 16.061 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.24 1367 CG ASP A 105 58.319 78.496 14.716 1.00 22.09 1369 OD2 ASP A 105 59.049 79.364 15.253 1.00 25.62 1370 C ASP A 105 54.851 79.525 16.069 1.00 25.92 1371 O ASP A 106 54.289 80.054 15.126 1.00 26.89 1374 CA ASP A 106 54.286 79.043 17.125 1.00 28.69 1374 CA							78.194	20.987		
1359 O MET A 104 57.213 81.186 17.942 1.00 25.54 1360 N ASP A 105 56.937 79.038 17.374 1.00 25.29 1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.24 1367 CG ASP A 105 58.819 78.496 14.716 1.00 24.83 1368 OD1 ASP A 105 58.853 77.642 13.954 1.00 22.09 1370 C ASP A 105 54.289 80.054 15.126 1.00 26.07 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 52.759 79.211 17.350 1.00 26.89 1374 CA ASP A 106 52.499 80.670 17.671 1.00 28.01 1375 CB						61.411	77.093	19.688	1.00	31.97
1360 N ASP A 105 56.937 79.038 17.374 1.00 25.29 1362 CA ASP A 105 56.373 79.388 16.061 1.00 25.81 1367 CG ASP A 105 56.832 78.449 14.969 1.00 25.24 1368 OD1 ASP A 105 58.853 77.642 13.954 1.00 22.09 1369 OD2 ASP A 105 59.049 79.364 15.253 1.00 25.62 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 52.759 79.211 17.350 1.00 27.69 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1374 CA </td <td>1358</td> <td>С</td> <td>MET</td> <td>Α</td> <td>104</td> <td>57.345</td> <td>79.995</td> <td>18.207</td> <td>1.00</td> <td>25.73</td>	1358	С	MET	Α	104	57.345	79.995	18.207	1.00	25.73
1362 CA ASP A 105 56.373 79.388 16.061 1.00 25.24 1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.24 1368 OD1 ASP A 105 58.319 78.496 14.716 1.00 22.09 1369 OD2 ASP A 105 59.049 79.364 15.253 1.00 25.62 1370 C ASP A 105 54.289 80.054 15.126 1.00 25.62 1371 O ASP A 106 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 52.759 79.211 17.350 1.00 27.69 1374 CA ASP A 106 52.419 80.670 17.671 1.00 28.12 1376 CB ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1<		0				57.213	81.186	17.942	1.00	25.54
1364 CB ASP A 105 56.832 78.419 14.969 1.00 25.24 1367 CG ASP A 105 58.319 78.496 14.716 1.00 24.83 1368 OD1 ASP A 105 58.853 77.642 13.954 1.00 22.09 1370 C ASP A 105 59.049 79.364 15.253 1.00 25.62 1371 O ASP A 105 54.851 79.525 16.069 1.00 26.07 1372 N ASP A 106 54.269 80.054 15.126 1.00 26.07 1374 CA ASP A 106 52.759 79.211 17.350 1.00 26.89 1374 CA ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 </td <td>1360</td> <td>N</td> <td>ASP</td> <td>Α</td> <td>105</td> <td>56.937</td> <td>79.038</td> <td>17.374</td> <td>1.00</td> <td>25.29</td>	1360	N	ASP	Α	105	56.937	79.038	17.374	1.00	25.29
1367 CG ASP A 105 58.319 78.496 14.716 1.00 24.83 1368 OD1 ASP A 105 58.853 77.642 13.954 1.00 22.09 1370 C ASP A 105 59.049 79.364 15.253 1.00 25.92 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.206 79.043 17.125 1.00 26.89 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 50.458 81.960 18.094 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05	1362	CA	ASP	Α	105	56.373	79.388	16.061	1.00	25.81
1368 OD1 ASP A 105 58.853 77.642 13.954 1.00 22.09 1369 OD2 ASP A 105 59.049 79.364 15.253 1.00 25.62 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.289 80.054 15.126 1.00 26.07 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 50.458 81.960 18.094 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 28.05 1381 OD2 ASP A 106 51.557	1364	CB	ASP	Α	105	56.832	78.419	14.969	1.00	25.24
1369 OD2 ASP A 105 59.049 79.364 15.253 1.00 25.62 1370 C ASP A 105 54.851 79.525 16.069 1.00 25.92 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 52.2759 79.211 17.350 1.00 27.69 1374 CA ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.76 1381 OD2 ASP A 106 51.952 78.715 16.157 1.00 28.07 1384 N ASP A 107 52.190 </td <td>1367</td> <td>CG</td> <td>ASP</td> <td>Α</td> <td>105</td> <td>58.319</td> <td>78.496</td> <td>14.716</td> <td>1.00</td> <td>24.83</td>	1367	CG	ASP	Α	105	58.319	78.496	14.716	1.00	24.83
1370 C ASP A 105 54.851 79.525 16.069 1.00 25.92 1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.206 79.043 17.125 1.00 26.89 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.07 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA <td>1368</td> <td>OD1</td> <td>ASP</td> <td>Α</td> <td>105</td> <td>58.853</td> <td>77.642</td> <td>13.954</td> <td>1.00</td> <td>22.09</td>	1368	OD1	ASP	Α	105	58.853	77.642	13.954	1.00	22.09
1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.206 79.043 17.125 1.00 26.89 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.592 78.715 16.157 1.00 28.05 1383 O ASP A 107 52.190 77.456 15.809 1.00 28.07 1384 N ASP A 107 51.534 76.822 14.686 1.00 25.66 <td>1369</td> <td>OD2</td> <td>ASP</td> <td>Α</td> <td>105</td> <td>59.049</td> <td>79.364</td> <td>15.253</td> <td>1.00</td> <td>25.62</td>	1369	OD2	ASP	Α	105	59.049	79.364	15.253	1.00	25.62
1371 O ASP A 105 54.289 80.054 15.126 1.00 26.07 1372 N ASP A 106 54.206 79.043 17.125 1.00 26.89 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 31.75 1381 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.05 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.05 1385 CA ASP A 107 52.553 76.822 14.686 1.00 25.56	1370	С	ASP	Α	105	54.851	79.525	16.069	1.00	25.92
1372 N ASP A 106 54.206 79.043 17.125 1.00 26.89 1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 100 31.76 1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 107 52.190 77.456 15.809 1.00 28.05 1384 N ASP A 107 51.534 76.822 14.686 1.00 27.99 1385 CB ASP A 107 53.069 76.830 12.677 1.00 25.56 <td>1371</td> <td>0</td> <td>ASP</td> <td>Α</td> <td>105</td> <td>54.289</td> <td>80.054</td> <td></td> <td>1.00</td> <td>26.07</td>	1371	0	ASP	Α	105	54.289	80.054		1.00	26.07
1374 CA ASP A 106 52.759 79.211 17.350 1.00 27.69 1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 51.952 78.715 16.157 1.00 28.05 1382 C ASP A 106 51.159 79.450 15.549 1.00 28.05 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 52.553 76.037 13.855 1.00 29.78 1391 CG ASP A 107 52.257 77.111 11.774 1.00 33.36 1392 OD1	1372	N	ASP	Α	106	54.206	79.043			
1376 CB ASP A 106 52.419 80.670 17.671 1.00 28.12 1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 107 52.190 77.456 15.549 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.2553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 52.2553 76.830 12.677 1.00 29.78 1392 O	1374	CA	ASP	Α						
1379 CG ASP A 106 51.000 80.840 18.202 1.00 29.63 1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.01 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.76 1393 OD2 ASP A 107 50.478 75.210 12.549 1.00 31.90	1376	СВ	ASP	Α	106					
1380 OD1 ASP A 106 50.458 81.960 18.094 1.00 31.75 1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.07 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 54.255 77.210 12.549 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP	1379	CG	ASP	Α		51.000				
1381 OD2 ASP A 106 50.342 79.911 18.732 1.00 31.76 1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.01 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 33.36 1393 OD2 ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 <										
1382 C ASP A 106 51.952 78.715 16.157 1.00 28.05 1383 O ASP A 106 51.159 79.450 15.549 1.00 28.01 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1398 CA ASP A 108 49.334 75.823 14.559 1.00 26.81 <td>1381</td> <td>OD2</td> <td>ASP</td> <td>Α</td> <td></td> <td>50.342</td> <td>79.911</td> <td></td> <td></td> <td></td>	1381	OD2	ASP	Α		50.342	79.911			
1383 O ASP A 106 51.159 79.450 15.549 1.00 28.01 1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 33.36 1393 OD2 ASP A 107 54.255 77.210 12.549 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 26.98 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1398 CA ASP A 108 49.334 75.823 14.559 1.00 26.81 1400 CB ASP A 108 46.929 75.778 15.08		C					78.715			
1384 N ASP A 107 52.190 77.456 15.809 1.00 28.07 1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.210 12.549 1.00 33.36 1393 OD2 ASP A 107 54.255 77.210 12.549 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1396 N ASP A 108 49.334 75.823 14.559 1.00 26.81 1400 CB ASP A 108 48.242 74.989 15.031 1.00 26.81 1403 CG ASP A 108 46.929 75.778 15.08	1383	0	ASP	Α	106			15.549		
1386 CA ASP A 107 51.534 76.822 14.686 1.00 27.99 1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 31.90 1394 C ASP A 107 50.478 75.822 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1396 N ASP A 108 49.334 75.823 14.559 1.00 26.95 1398 CA ASP A 108 48.242 74.989 15.031 1.00 26.81 1400 CB ASP A 108 46.929 75.778 15.089 1.00 27.66 1403 CG ASP A 108 46.453 76.241 13.725 1.00 30.37 </td <td>1384</td> <td>N</td> <td>ASP</td> <td>Α</td> <td></td> <td>52.190</td> <td></td> <td></td> <td></td> <td></td>	1384	N	ASP	Α		52.190				
1388 CB ASP A 107 52.553 76.037 13.855 1.00 28.56 1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 33.36 1393 OD2 ASP A 107 54.255 77.210 12.549 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1396 N ASP A 108 49.334 75.823 14.559 1.00 26.95 1398 CA ASP A 108 48.242 74.989 15.031 1.00 26.81 1400 CB ASP A 108 46.929 75.778 15.089 1.00 27.66 1403 CG ASP A 108 46.453 76.241 13.725 1.00 30.37 1404 OD1 ASP A 108 47.165 76.194 12.690 1.00 32.04<	1386	CA			107					
1391 CG ASP A 107 53.069 76.830 12.677 1.00 29.78 1392 OD1 ASP A 107 52.257 77.111 11.774 1.00 33.36 1393 OD2 ASP A 107 54.255 77.210 12.549 1.00 31.90 1394 C ASP A 107 50.478 75.882 15.230 1.00 27.64 1395 O ASP A 107 50.693 75.218 16.248 1.00 26.98 1396 N ASP A 108 49.334 75.823 14.559 1.00 26.95 1398 CA ASP A 108 48.242 74.989 15.031 1.00 26.81 1400 CB ASP A 108 46.929 75.778 15.089 1.00 27.66 1403 CG ASP A 108 46.453 76.241 13.725 1.00 30.37 1404 OD1 ASP A 108 45.282 76.700 13.645 1.00 33.61 1405 OD2 ASP A 108 47.165 76.194 12.690 1.00 25.76	1388	CB	ASP	Α			76.037			
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1412 CB LEU A 109 48.106 72.694 10.945 1.00 25.33 1415 CG LEU A 109 46.598 72.821 10.810 1.00 26.83										
1415 CG LEU A 109 46.598 72.821 10.810 1.00 26.83										
1417 CD1 LEU A 109 46.260 73.283 9.399 1.00 29.44										
1421 CD2 LEU A 109 45.903 71.492 11.089 1.00 27.95										

FIGURE 3 (Cont.)AO

1425 C LEU A 109	A	В	С	D	E	F	G	Н	I	J
1426 O	1425	С	LEU	Α	109	50.144	71.781	12.034	1.00	23.64
1427 N ARG A 110 50.237 70.454 12.081 1.00 22.79 1429 CA ARG A 110 51.401 69.715 11.603 1.00 22.20 14341 CB ARG A 110 52.479 69.644 12.672 1.00 21.90 1434 CG ARG A 110 52.479 69.644 12.672 1.00 21.96 1437 CD ARG A 110 54.820 68.975 13.195 1.00 21.16 1440 NE ARG A 110 55.377 70.290 13.472 1.00 12.55 1442 CZ ARG A 110 55.377 70.290 13.472 1.00 12.55 1442 NH1 ARG A 110 56.777 70.290 12.721 1.00 21.19 1443 NH1 ARG A 110 56.740 72.082 13.111 1.00 21.59 1444 NH2 ARG A 110 56.737 70.355 11.590 1.00 21.98 1449 C ARG A 110 50.997 68.301 11.215 1.00 22.79 1451 N ARG A 110 50.997 68.301 11.215 1.00 22.79 1453 CA ARG A 111 51.566 67.807 10.122 1.00 22.79 1453 CA ARG A 111 51.566 67.807 10.122 1.00 22.79 1453 CA ARG A 111 51.814 65.407 10.477 1.00 23.33 1458 CG ARG A 111 53.310 65.424 10.531 1.00 21.59 1464 NE ARG A 111 55.237 66.489 9.580 1.00 23.42 1464 NE ARG A 111 55.3310 65.424 10.531 1.00 21.59 1464 NE ARG A 111 55.282 64.632 11.726 1.00 21.03 1467 NH1 ARG A 111 55.486 63.657 10.0477 10.00 23.33 1466 CZ ARG A 111 55.486 63.576 13.760 1.00 21.59 1470 NH2 ARG A 111 55.486 67.387 9.374 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 22.79 1474 O ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.733 66.284 9.374 1.00 24.49 1475 N GLY A 112 47.641 67.363 8.673 1.00 24.90 1475 N GLY A 112 47.641 67.363 8.673 1.00 24.90 1480 C GLY A 112 47.641 67.363 8.673 1.00 24.90 1481 O GLY A 112 46.709 67.432 9.854 1.00 27.01 1486 CB LEU A 113 46.38 64.99 12.230 1.00 27.29 1491 CD1 LEU A 113 46.78 67.425 12.301 1.00 27.29 1499 C LEU A 113 46.78 67.425 12.301 1.00 27.29 1499 C LEU A 113 46.78 67.425 12.301 1.00 27.29 1499 C LEU A 113 46.78 67.425 12.301 1.00 26.97 1500 O LEU A 113 46.78 67.425 12.301 1.00 26.97 1501 N PRO A 114 46.942 69.737 15.341 1.00 26.97 1502 CA PRO A 114 46.942 69.737 15.636 1.00 27.01 1510 CD PRO A 114 46.942 69.737 15.636 1.00 27.03 1510 CD PRO A 114 47.988 68.247 16.088 1.00 27.01 1510 CD PRO A 114 47.988 68.247 16.088 1.00 25.67 1521 OG1 THR A 115 50.901 72.085 15.422 1.00 25.77 1527 C THR A 115										
1429 CA ARG A 110										
1431 CB ARG A 110 52.479 69.644 12.672 1.00 21.90 1434 CG ARG A 110 55.742 69.015 12.166 1.00 21.62 1.63 1437 CD ARG A 110 55.820 68.975 13.195 1.00 21.16 1440 NE ARG A 110 55.377 70.290 13.472 1.00 19.55 1442 CZ ARG A 110 56.740 72.082 13.111 1.00 21.55 1446 NH2 ARG A 110 56.740 72.082 13.111 1.00 21.55 1446 NH2 ARG A 110 56.740 72.082 13.111 1.00 21.57 1449 C ARG A 110 56.740 72.082 13.111 1.00 21.57 1445 N ARG A 110 50.997 68.301 11.215 1.00 21.87 1451 N ARG A 110 50.997 68.301 11.215 1.00 22.99 1453 CA ARG A 111 51.566 67.807 10.122 1.00 22.79 1453 CA ARG A 111 51.566 67.807 10.122 1.00 22.79 1453 CA ARG A 111 51.237 66.489 9.580 1.00 23.42 1455 CB ARG A 111 55.310 65.424 10.531 1.00 21.59 1466 CZ ARG A 111 55.3310 65.424 10.531 1.00 21.59 1466 CZ ARG A 111 55.282 64.632 11.726 1.00 21.03 1467 NH1 ARG A 111 55.486 63.576 13.760 1.00 27.55 1470 NH2 ARG A 111 55.486 63.576 13.760 1.00 20.75 1470 NH2 ARG A 111 55.486 67.387 13.950 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 22.79 1475 N GLY A 112 49.048 67.375 9.037 1.00 22.79 1475 N GLY A 112 49.048 67.375 9.037 1.00 22.79 1475 N GLY A 112 49.048 67.375 9.037 1.00 22.79 1488 CG LEU A 113 46.709 67.432 9.854 1.00 27.06 1488 N LEU A 113 46.786 67.363 8.673 1.00 26.45 1488 CG LEU A 113 46.786 67.363 8.673 1.00 27.66 1488 N LEU A 113 46.786 67.375 9.037 1.00 27.66 1488 N LEU A 113 46.786 67.375 9.037 1.00 27.66 1488 CG LEU A 113 46.786 67.375 9.037 1.00 27.66 1488 CG LEU A 113 46.786 67.375 9.037 1.00 27.66 1489 CG LEU A 113 46.786 67.363 8.673 1.00 27.66 1489 CG LEU A 113 46.786 67.383 9.653 1.00 27.66 1488 CG LEU A 113 46.786 67.383 9.8563 1.00 27.66 1488 CG LEU A 113 46.786 67.385 9.285 1.00 27.61 1.00 27.18 1486 CB LEU A 113 46.786 67.385 9.285 1.00 27.61										
1434 CG ARG A 110 54.820 68.975 13.195 1.00 21.62 1440 NE ARG A 110 54.820 68.975 13.195 1.00 21.16 1440 NE ARG A 110 55.377 70.290 12.721 1.00 21.15 1442 CZ ARG A 110 56.737 70.905 12.721 1.00 21.15 1443 NHL ARG A 110 56.737 70.355 11.590 1.00 21.98 1445 O ARG A 110 50.997 68.301 11.215 1.00 21.97 1455 O ARG A 111 51.566 67.807 10.122 1.00 22.97 1455 CA ARG A 111 51.584 65.407 10.122 1.00 23.42 1455 CB ARG A 111 51.846 <td></td>										
1437 CD ARG A 110 54.820 68.975 13.195 1.00 21.16 1440 NE ARG A 110 55.377 70.290 13.472 1.00 21.51 1443 NH1 ARG A 110 56.777 70.905 12.721 1.00 21.95 1446 NH2 ARG A 110 56.777 70.355 11.590 1.00 21.98 1450 O ARG A 110 50.787 70.355 11.590 1.00 21.98 1451 O ARG A 110 50.184 67.686 11.876 1.00 22.79 1453 CA ARG A 111 51.266 67.807 10.122 1.00 23.42 1455 CB ARG A 111 51.814 65.407 10.476 1.00 22.10 1466 NE ARG A 111 53.841 </td <td></td>										
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1455 CB ARG A 111 51.814 65.407 10.477 1.00 23.33 1458 CG ARG A 111 53.310 65.424 10.531 1.00 22.10 1464 NE ARG A 111 55.282 64.632 11.726 1.00 21.03 1466 CZ ARG A 111 55.282 64.632 11.726 1.00 21.03 1470 NH1 ARG A 111 55.438 63.576 13.760 1.00 20.75 1470 NH2 ARG A 111 57.323 64.020 12.544 1.00 22.79 1473 C ARG A 111 49.216 65.181 9.528 1.00 24.99 1477 CA GLY 112 47.641 67.363 8.673 1.00 25.84 1477 CA GLY 112 46.709 67.322 <th< td=""><td>1453</td><td>CA</td><td>ARG</td><td>A</td><td></td><td></td><td></td><td></td><td></td><td></td></th<>	1453	CA	ARG	A						
1458 CG ARG A 111 53.310 65.424 10.531 1.00 22.10 1461 CD ARG A 111 53.841 64.752 11.768 1.00 21.59 1464 NE ARG A 111 55.282 64.632 11.726 1.00 21.01 1466 CZ ARG A 111 55.438 63.576 13.760 1.00 20.75 1470 NH2 ARG A 111 55.438 63.576 13.760 1.00 20.75 1473 C ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.216 65.181 9.528 1.00 24.99 1477 CA GLY A 112 47.641 67.363 8.673 1.00 25.84 1477 CA GLY A 112 45.500		CB	ARG	Α						
1461 CD ARG A 111 53.841 64.752 11.768 1.00 21.59 1464 NE ARG A 111 55.282 64.632 11.768 1.00 21.10 1466 CZ ARG A 111 55.282 64.632 11.768 1.00 21.01 1467 NH1 ARG A 111 55.438 63.576 13.760 1.00 20.75 1470 NH2 ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.216 65.181 9.528 1.00 24.99 1475 N GLY A 112 47.641 67.363 8.673 1.00 25.84 1480 C GLY A 112 47.641 67.363 8.673 1.00 27.01 1481 O GLY A 112 45.500	1458		ARG	Α						
1464 NE ARG A 111 55.282 64.632 11.726 1.00 21.10 1466 CZ ARG A 111 56.009 64.082 12.681 1.00 21.03 1467 NH1 ARG A 111 55.438 63.576 13.760 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.216 65.181 9.528 1.00 24.99 1475 N GLY A 112 49.048 67.375 9.037 1.00 25.84 1477 CA GLY A 112 46.709 67.432 9.854 1.00 27.01 1480 C GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 46.478	1461	CD	ARG	Α					1.00	21.59
1467 NH1 ARG A 111 55.438 63.576 13.760 1.00 20.75 1470 NH2 ARG A 111 57.323 64.020 12.544 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.216 65.181 9.528 1.00 24.90 1475 N GLY A 112 49.048 67.375 9.037 1.00 26.45 1480 C GLY A 112 47.641 67.363 8.673 1.00 27.01 1481 O GLY A 112 46.709 67.432 9.854 1.00 27.06 1482 N LEU A 113 47.258 67.574 11.066 1.00 27.18 1484 CA LEU A 113 46.478 67.445 12.301 1.00 27.26 1489 CG LEU	1464	NE	ARG	Α	111	55.282	64.632			21.10
1470 NH2 ARG A 111 57.323 64.020 12.544 1.00 22.79 1473 C ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.048 67.375 9.037 1.00 25.84 1477 CA GLY A 112 47.641 67.363 8.673 1.00 26.45 1480 C GLY A 112 46.709 67.432 9.854 1.00 27.01 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 46.478 67.574 11.066 1.00 27.18 1485 CB LEU A 113 46.478 67.445 12.301 1.00 27.29 1489 CG LEU A 113 46.96	1466	CZ	ARG	Α	111	56.009	64.082	12.681	1.00	21.03
1473 C ARG A 111 49.733 66.284 9.374 1.00 24.49 1474 O ARG A 111 49.216 65.181 9.528 1.00 24.90 1475 N GLY A 112 49.048 67.375 9.037 1.00 25.84 1477 CA GLY A 112 47.641 67.363 8.673 1.00 26.45 1480 C GLY A 112 45.500 67.432 9.854 1.00 27.01 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.796	1467	NH1	ARG	Α	111	55.438	63.576	13.760	1.00	20.75
1474 O ARG A 111 49.216 65.181 9.528 1.00 24.90 1475 N GLY A 112 49.048 67.375 9.037 1.00 25.84 1477 CA GLY A 112 47.641 67.363 8.673 1.00 26.45 1480 C GLY A 112 45.500 67.432 9.854 1.00 27.06 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.783 68.4849 12.230 1.00 29.25 1491 CD1 LEU A 113 46.793	1470	NH2	ARG	Α	111	57.323	64.020	12.544	1.00	22.79
1475 N GLY A 112 49.048 67.375 9.037 1.00 25.84 1477 CA GLY A 112 47.641 67.363 8.673 1.00 26.45 1480 C GLY A 112 46.709 67.432 9.854 1.00 27.01 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 47.258 67.574 11.066 1.00 27.29 1486 CB LEU A 113 46.478 67.445 12.301 1.00 27.29 1488 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799	1473	C	ARG	Α	111	49.733	66.284	9.374	1.00	24.49
1477 CA GLY A 112 47.641 67.363 8.673 1.00 26.45 1480 C GLY A 112 46.709 67.432 9.854 1.00 27.01 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 47.258 67.574 11.066 1.00 27.29 1486 CB LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.956 63.639 12.826 1.00 29.25 1491 CD1 LEU A 113 44.799 64.723 12.297 1.00 26.95 1500 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.97 1502	1474	0	ARG	Α	111	49.216	65.181	9.528	1.00	24.90
1480 C GLY A 112 46.709 67.432 9.854 1.00 27.01 1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 47.258 67.574 11.066 1.00 27.29 1486 CB LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.25 1491 CD1 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.93	1475	N	\mathtt{GLY}	Α	112	49.048	67.375	9.037	1.00	25.84
1481 O GLY A 112 45.500 67.383 9.663 1.00 27.66 1482 N LEU A 113 47.258 67.574 11.066 1.00 27.18 1484 CA LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.40 1495 CD2 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 45.151 69.465 16.391<	1477	CA	GLY	Α	112	47.641	67.363	8.673	1.00	26.45
1482 N LEU A 113 47.258 67.574 11.066 1.00 27.18 1484 CA LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.40 1495 CD2 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 45.151 69.465 16.391 1.00 26.39 </td <td>1480</td> <td>C</td> <td>GLY</td> <td>Α</td> <td>112</td> <td>46.709</td> <td>67.432</td> <td>9.854</td> <td>1.00</td> <td>27.01</td>	1480	C	GLY	Α	112	46.709	67.432	9.854	1.00	27.01
1484 CA LEU A 113 46.478 67.445 12.301 1.00 27.29 1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.25 1491 CD1 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.03 <	1481	0	\mathtt{GLY}	Α	112	45.500	67.383	9.663	1.00	27.66
1486 CB LEU A 113 46.778 66.104 12.965 1.00 27.61 1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.25 1491 CD1 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.03 1513 C <td>1482</td> <td>N</td> <td>LEU</td> <td>Α</td> <td></td> <td>47.258</td> <td></td> <td>11.066</td> <td>1.00</td> <td>27.18</td>	1482	N	LEU	Α		47.258		11.066	1.00	27.18
1489 CG LEU A 113 46.308 64.849 12.230 1.00 29.25 1491 CD1 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.42 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 47.644 69.428 15.902 1.00 25.96 <	1484	CA	LEU	A	113	46.478	67.445	12.301	1.00	27.29
1491 CD1 LEU A 113 46.956 63.639 12.826 1.00 29.40 1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088	1486		LEU	Α		46.778	66.104		1.00	27.61
1495 CD2 LEU A 113 44.799 64.723 12.297 1.00 30.33 1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 49.730 70.336 16.803 </td <td>1489</td> <td></td> <td></td> <td></td> <td>113</td> <td>46.308</td> <td></td> <td>12.230</td> <td>1.00</td> <td>29.25</td>	1489				113	46.308		12.230	1.00	29.25
1499 C LEU A 113 46.783 68.580 13.279 1.00 26.95 1500 O LEU A 113 47.781 69.273 13.134 1.00 26.97 1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 49.730 70.336 16.803 1.00 25.63 1519 CB THR A 115 49.605 72.715 17.288 <td>1491</td> <td></td> <td></td> <td></td> <td></td> <td>46.956</td> <td>63.639</td> <td>12.826</td> <td>1.00</td> <td>29.40</td>	1491					46.956	63.639	12.826	1.00	29.40
1500 O LEU A 113	1495				113	44.799		12.297	1.00	30.33
1501 N PRO A 114 45.911 68.807 14.256 1.00 26.77 1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 49.605 72.715 17.288 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89		С								26.95
1502 CA PRO A 114 46.242 69.737 15.341 1.00 26.42 1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 49.730 70.336 16.803 1.00 25.53 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										26.97
1504 CB PRO A 114 45.151 69.465 16.391 1.00 26.39 1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1507 CG PRO A 114 43.997 68.927 15.636 1.00 27.10 1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 24.78 </td <td></td>										
1510 CD PRO A 114 44.540 68.278 14.377 1.00 27.03 1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 25.67 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1513 C PRO A 114 47.644 69.428 15.902 1.00 25.96 1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 25.67 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1514 O PRO A 114 47.988 68.247 16.088 1.00 25.12 1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1515 N THR A 115 48.433 70.470 16.131 1.00 25.63 1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1517 CA THR A 115 49.730 70.336 16.803 1.00 25.53 1519 CB THR A 115 50.478 71.668 16.835 1.00 25.67 1521 OG1 THR A 115 49.605 72.715 17.288 1.00 26.41 1523 CG2 THR A 115 50.901 72.085 15.442 1.00 25.77 1527 C THR A 115 49.531 69.838 18.228 1.00 25.27 1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
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1528 O THR A 115 48.430 69.941 18.787 1.00 24.78 1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
1529 N CYS A 116 50.600 69.305 18.817 1.00 24.89										
	1531	CA			116	50.523	68.697	20.137		

FIGURE 3 (Cont.) AP

A	В	С	D	E	F	G	Н	I	J
1533	СВ	CYS	Α	116	51.895	68.165	20.581	1.00	24.90
1536	SG	CYS		116	52.285	66.565	19.821		24.91
1537	C	CYS		116	49.933	69.634	21.182	1.00	24.97
1538	ō	CYS		116	49.096	69.228	21.971	1.00	24.71
1539	N	HIS		117	50.346	70.894	21.168	1.00	25.78
1541	CA	HIS		117	49.925	71.820	22.208	1.00	26.16
1543	CB	HIS		117	50.836	73.054	22.246	1.00	26.51
1546	CG	HIS		117	50.548	74.067	21.186	1.00	
1547	ND1		A	117	50.785	73.840	19.849	1.00	30.89
1549	CEI		A	117	50.441	74.911	19.156	1.00	30.52
1551	NE2		A	117	50.007	75.831	19.136		30.35
1553		HIS		117	50.066	75.327	21.272	1.00	29.44
1555	C	HIS		117	48.433	72.162	22.054		26.69
1556	0	HIS		117	40.433				
1557	N	VAL				72.385	23.040		26.52
				118	47.938	72.180	20.820	1.00	
1559	CA	VAL		118	46.510	72.380	20.577		27.86
1561	CB	VAL		118	46.217	72.617	19.078		27.70
1563	CG1	VAL		118	44.701	72.510	18.774		28.86
1567	CG2	VAL		118	46.737	73.972	18.645		28.14
1571	C	VAL		118	45.695	71.196	21.131	1.00	28.24
1572	0	VAL		118	44.784	71.396	21.935	1.00	28.47
1573	N	LYS		119	46.040	69.973	20.733		28.54
1575	CA	LYS		119	45.245	68.798	21.101		29.34
1577	CB	LYS		119	45.617	67.583	20.241		29.61
1580	CG	LYS		119	44.863	66.301	20.626	1.00	30.82
1583	CD	LYS		119	45.106	65.186	19.627	1.00	32.53
1586	CE	LYS		119	44.199	63.976	19.839	1.00	33.76
1589	NZ	LYS		119	43.344	64.050	21.054	1.00	36.05
1593	C	LYS		119	45.371	68.422	22.581	1.00	
1594	0		A	119	44.383	68.012	23.194		29.82
1595	N	PHE	Α	120	46.575	68.551	23.146	1.00	28.84
1597	CA		Α	120	46.839	68.108	24.519	1.00	28.62
1599	CB	PHE		120	47.984	67.096	24.529	1.00	28.31
1602	CG		Α	120	47.722	65.880	23.711		27.28
1603	CD1	PHE	Α	120	47.055	64.787	24.261		27.38
1605	CE1		Α	120	46.831	63.631	23.508		27.16
1607	CZ	PHE		120	47.271	63.563	22.198		27.58
1609		PHE		120	47.932	64.648	21.636		27.23
1611	CD2	PHE		120	48.163	65.804	22.399		27.44
1613	C	PHE		120	47.185	69.217	25.515		28.26
1614	0	PHE		120	47.341	68.943	26.706		29.25
1615	N	GLY		121	47.299	70.452	25.042	1.00	27.60
1617	CA	GLY		121	47.659	71.575	25.896		26.94
1620	С	GLY		121	49.155	71.840	25.860		26.46
1621	0	GLY		121	49.958	70.992	25.438		26.06
1622	N	GLU		122	49.536	73.009	26.340		25.72
1624	CA	GLU		122	50.910	73.462	26.248		25.58
1626	CB	GLU		122	51.007	74.958	26.519		25.87
1629	CG	GLU		122	50.483	75.783	25.358		29.11
1632	CD	GLU		122	50.355	77.241	25.698		33.26
1633		GLU		122	51.247	77.754	26.399		35.51
1634	OE2	GLU	Α	122	49.349	77.861	25.269	1.00	37.97

FIGURE 3 (Cont.)AQ

Α	В	С	D	E	F	G	Н	I	J
1635	С	GLU	Α	122	51.798	72.689	27.211	1.00	24.80
1636	o	GLU		122	52.899	72.300	26.840		24.40
1637	N	ALA		123	51.320	72.474	28.436		23.77
1639	CA	ALA		123	52.098	71.760	29.447		23.73
1641	CB	ALA	A	123	51.353	71.711	30.776		23.98
1645	С	ALA	Α	123	52.441	70.343	28.968	1.00	23.81
1646	0	ALA	Α	123	53.603	69.943	29.024	1.00	24.19
1647	N	ASN	Α	124	51.442	69.609	28.479	1.00	22.86
1649	CA	ASN	Α	124	51.654	68.270	27.947	1.00	22.86
1651	CB	ASN	Α	124	50.345	67.623	27.491	1.00	23.02
1654	CG	ASN	Α	124	49.539	67.041	28.635	1.00	24.68
1655	OD1	ASN	A	124	48.304	67.110	28.640	1.00	27.85
1656	ND2	ASN		124	50.220	66.461	29.600	1.00	25.67
1659	C	ASN		124	52.631	68.261	26.779	1.00	21.84
1660	0	ASN		124	53.428	67.339	26.667	1.00	
1661	N	ALA		125	52.543	69.263	25.908	1.00	20.33
1663	CA	ALA		125	53.457	69.399	24.788	1.00	20.39
1665	CB	ALA		125	52.984	70.529	23.886	1.00	
1669	C	ALA		125	54.925	69.621	25.250	1.00	19.95
1670	0	ALA		125	55.856	68.974	24.760	1.00	19.97
1671	N	ILE		126	55.117	70.509	26.218	1.00	19.41
1673	CA	ILE		126	56.434	70.769	26.790	1.00	19.39
1675	CB	ILE		126	56.357	71.842	27.880	1.00	19.07
1677 1680	CG1 CD1	ILE		126 126	56.032	73.214	27.267	1.00	20.58
1684	CG2	ILE		126	55.450 57.668	74.180 71.944	28.244	1.00	22.11 19.77
1688	C	ILE		126	57.000	69.487	28.623 27.378	1.00	19.77
1689	0	ILE		126	58.134	69.105	27.069	1.00	18.97
1690	N	LEU		127	56.229	68.824	28.211	1.00	18.52
1692	CA	LEU		127	56.694	67.637	28.913	1.00	19.19
1694	СВ	LEU		127	55.716	67.252	30.029	1.00	19.06
1697	CG	LEU		127	55.616	68.280	31.166	1.00	20.37
1699	CD1	LEU		127	56.961	68.500	31.859	1.00	22.60
1703	CD2	LEU		127	54.595	67.820	32.159	1.00	21.48
1707	С	LEU	Α	127	56.907	66.470	27.966	1.00	18.53
1708	0	LEU	Α	127	57.856	65.723	28.126	1.00	18.41
1709	N	ALA	Α	128	56.033	66.320	26.973	1.00	17.92
1711	CA	ALA	Α	128	56.179	65.228	26.012	1.00	17.62
1713	CB	ALA	Α	128	54.947	65.115	25.104	1.00	17.67
1717	С	ALA		128	57.434	65.418	25.168	1.00	17.09
1718	0	АĻА		128	58.108	64.461	24.828	1.00	17.12
1719	N	GLY		129	57.740	66.649	24.807	1.00	16.81
1721	CA	GLY		129	58.945	66.914	24.059	1.00	16.96
1724	C	GLY		129	60.155	66.651	24.946	1.00	17.30
1725	0	GLY		129	61.102	66.022	24.500	1.00	17.59
1726	N	ASP		130	60.106	67.121	26.193	1.00	17.16
1728	CA	ASP		130	61.139	66.853	27.190	1.00	17.77
1730	CB	ASP		130	60.717	67.383	28.562	1.00	18.20
1733 1734	CG OD1	ASP ASP		130	60.801 61.407	68.881	28.661 27.759	1.00	19.18
1735		ASP		130 130	60.295	69.492 69.527	29.612		21.99 19.91
1736	C C	ASP		130	61.410	65.359	27.301		17.64
1,30	_	AUP	~	200	01.410	55.55	21.301	1.00	11.04

FIGURE 3 (Cont.) AR

A	В	С	D	E	F	G	Н	I	J
1737	0	ASP	Δ	130	62.548	64.927	27.230	1.00	17.90
1738	N	ALA		131	60.343	64.584	27.230	1.00	17.42
1740	CA	ALA		131	60.438	63.146	27.633	1.00	17.39
1742	CB	ALA		131	59.098	62.582	28.089	1.00	17.97
1746	C	ALA		131	60.910	62.429	26.378	1.00	17.06
1747	0	ALA		131	61.576	61.425	26.378	1.00	16.51
1748	N	LEU		132	60.525	62.918	25.197	1.00	17.23
1750	CA	LEU		132	61.005	62.333	23.197	1.00	17.60
1752	CB	LEU		132		62.333			
1755	CG	LEU		132	60.265	62.247	22.740	1.00	17.59
1757	CD1	LEU		132	58.930		22.427	1.00	17.08
1761	CD1	LEU		132	58.170	63.044	21.399	1.00	18.87
	CDZ				59.126	60.798	21.970	1.00	18.78
1765		LEU		132	62.515	62.534	23.779	1.00	17.74
1766 1767	N O	LEU GLN		132	63.197	61.641	23.297	1.00	17.61
				133	63.036	63.695	24.185	1.00	17.96
1769 1771	CA	GLN		133	64.483	63.926	24.148	1.00	18.23
	CB	GLN GLN		133	64.894	65.366	24.559	1.00	18.28
1774	CG			133	66.427	65.512	24.520	1.00	19.50
1777	CD	GLN		133	67.021	66.816	25.074	1.00	22.38
1778	OE1	GLN		133	66.350	67.833	25.237	1.00	19.65
1779	NE2	GLN		133	68.322	66.768	25.346	1.00	23.26
1782	C	GLN		133	65.165	62.906	25.043	1.00	17.62
1783	0	GLN		133	66.132	62.284	24.645	1.00	17.06
1784	N	THR		134	64.650	62.736	26.258	1.00	18.05
1786	CA	THR		134	65.220	61.790	27.201	1.00	18.07
1788	CB	THR		134	64.461	61.797	28.520	1.00	18.89
1790	OG1	THR		134	64.445	63.109	29.073	1.00	17.91
1792	CG2	THR		134	65.189	60.940	29.551	1.00	18.65
1796	C	THR		134	65.165	60.373	26.665	1.00	17.74
1797	0	THR		134	66.111	59.615	26.829	1.00	17.70
1798	N	LEU		135	64.056	60.037	26.016	1.00	17.32
1800	CA	LEU		135	63.863	58.698	25.487	1.00	17.21
1802	CB	LEU		135	62.450	58.554	24.899	1.00	16.68
1805	CG	LEU		135	62.102	57.160	24.360	1.00	17.14
1807	CD1	LEU		135	62.252	56.096	25.413	1.00	17.24
1811	CD2 C	LEU		135	60.691	57.141	23.772	1.00	17.71
1815		LEU		135	64.934	58.362	24.443	1.00	16.99
1816	0	LEU ALA		135 136	65.396	57.234	24.373		17.51
1817	N				65.311	59.345	23.637		16.86
1819	CA CB	ALA		136	66.350	59.191	22.640	1.00	
1821		ALA		136	66.617	60.525	21.936	1.00	16.96
1825	C	ALA		136	67.629	58.656	23.286	1.00	17.44
1826	O N	ALA		136	68.269	57.772	22.741		17.77
1827		PHE		137	67.982	59.193	24.449		17.78
1829	CA CB	PHE		137	69.179	58.770	25.172	1.00	
1831 1834	CG	PHE PHE		137 137	69.700 70.113	59.891 61.073	26.062 25.279	1.00	18.06 18.66
1835	CD1	PHE		137	69.308	62.203		1.00	
1837	CE1	PHE		137	69.672	62.203	25.215 24.422	1.00	17.95
1839	CZ	PHE		137	70.834	63.284	24.422		18.78 18.81
1841	CE2	PHE		137	70.634	62.108	23.669		19.03
1843		PHE		137	71.047	61.031	24.526		19.55
1043	CDZ	4114	_	±3 /	11.211	J1. UJ1	24.320	1.00	19.55

FIGURE 3 (Cont.) AS

A	В	С	D	E	F		G		H .	I		J
1845	С	PHE	Α	137	69.	000	57.481		25.944	1.0	0.0	17.78
1846	Ō	PHE		137	69.		56.741		26.093	1.0		19.01
1847	N	SER		138	67.		57.181		26.383	1.0		17.63
1849	CA			138	67.		55.853		26.930	1.0		17.81
1851	CB	SER	Α	138	66.		55.790		27.503	1.0		18.14
1854	OG	SER		138	65.		56.474		28.749	1.0		19.62
1856	С	SER	Α	138	67.		54.788		25.860	1.0		17.61
1857	0	SER	Α	138	68.	139	53.706	; ;	26.127	1.0	00	17.31
1858	N	ILE	Α	139	67.	202	55.100	:	24.646	1.0	0	17.34
1860	CA	ILE	Α	139	67.	275	54.150) ;	23.545	1.0	0	18.07
1862	CB	ILE	Α	139	66.	528	54.676		22.286	1.0	0	18.17
1864	CG1	ILE	Α	139	65.	001	54.638		22.531	1.0	0	18.76
1867	CD1	ILE	Α	139	64.	188	55.429) ;	21.499	1.0	0	19.79
1871	CG2	ILE	Α	139	66.	878	53.836		21.073	1.0	0	19.10
1875	С	ILE		139	68.	732	53.827	' :	23.237	1.0	0	17.54
1876	0	ILE		139	69.	102	52.663	. :	23.207	1.0	0	17.29
1877	N	LEU	Α	140	69.	556	54.854	:	23.081	1.0	0	17.52
1879	CA	LEU	Α	140	70.		54.677	' :	22.710	1.0	0	18.26
1881	CB	LEU		140	71.	607	56.028		22.388	1.0	0	18.48
1884	CG	LEU		140	71.		56.649		21.066	1.0	0	18.76
1886	CD1	LEU		140	71.		57.952		20.786	1.0	0	19.92
1890	CD2	LEU		140	71.		55.663		19.939	1.0	0	19.54
1894	С	LEU		140	71.		53.986		23.786	1.0		18.96
1895	0	LEU		140	72.		53.265		23.476	1.0		18.14
1896	N	SER		141	71.		54.201		25.046	1.0		19.45
1898	CA	SER		141	72.		53.596		26.142	1.0		20.52
1900	CB	SER		141	72.		54.482		27.404	1.0		20.39
1903	OG	SER		141	70.		54.763		27.813	1.0		22.72
1905	C	SER		141	71.		52.157		26.439	1.0		20.99
1906	0	SER	A	141	72.		51.344		26.874	1.0		21.12
1907	N C?	ASP	A	142	70.		51.840		26.157	1.0		20.94
1909	CA	ASP ASP	A	142	69.		50.583		26.617	1.0		21.52
1911 1914	CB CG	ASP	A A	142 142	68.		50.885		27.360 28.668	1.0		21.35
1915	OD1	ASP	A	142	68. 67.		51.573			1.0		23.16
1916	OD1		A	142	67. 69.		52.038 51.678		29.261 29.188	1.0		22.75 24.41
1917	C	ASP		142	69.		49.569		25.557	1.0		21.65
1918	0	ASP		142	69.		48.382		25.850			20.45
1919	N	ALA		143	69.		50.033		24.342			22.42
1921	CA	ALA		143	68.		49.176		23.301			23.31
1923	СВ	ALA		143	68.		50.004		22.165			22.74
1927	C	ALA		143	69.		48.200		22.795			24.09
1928	0	ALA		143	70.		48.453		22.888			24.03
1929	N	ASP		144	69.		47.087		22.256			25.84
1931	CA	ASP		144	70.		46.051		21.707			27.11
1933	CB	ASP		144	69.		44.768		21.402			27.68
1936	CG	ASP		144	68.		44.426		22.469	1.0		31.56
1937	OD1	ASP		144	67.		44.829		22.309	1.0		38.25
1938	OD2	ASP	Α	144	68.	558	43.752		23.487			35.92
1939	С	ASP		144	70.	716	46.563		20.420	1.0		26.94
1940	0	ASP		144	69.	995	46.966		19.504	1.0	0	27.42
1941	N	MET	A	145	72.	044	46.586		20.374	1.0	0	27.00

FIGURE 3 (Cont.) AT

Α	В	С	D	E	F	G	Н	I	J
			_						
1943	CA	MET		145	72.794	46.828	19.148	1.00	27.40
1945	CB	MET		145	73.297	48.273	19.105	1.00	27.32
1948	CG			145	72.199	49.301	19.048	1.00	27.17
1951	SD			145	72.806	50.970	18.731	1.00	27.97
1952	CE	MET	A	145	73.747	51.294	20.169	1.00	26.35
1956	C	MET	A	145	73.972	45.850	19.125	1.00	28.08
1957	0	MET	A	145	75.099	46.213	19.487	1.00	27.86
1958	N			146	73.702	44.596	18.768	1.00	28.99
1959	CA	PRO		146	74.700	43.519	18.900	1.00	29.80
1961	CB	PRO		146	74.018	42.301	18.244	1.00	30.17
1964	CG	PRO		146	72.730	42.788	17.654	1.00	
1967	CD	PRO		146	72.402	44.090	18.296	1.00	29.22
1970	С 0	PRO		146	76.088	43.778	18.280	1.00	29.90
1971 1972	N	PRO GLU		146 147	77.081 76.176	43.394	18.874	1.00	30.77
1974	CA	GLU		147	77.488	44.452 44.605	17.149 16.495	1.00	30.07
1976	CB	GLU		147		44.666	14.970	1.00	30.29
1979	CG	GLU		147	77.348 76.419	43.625	14.368	1.00	33.60
1982	CD	GLU		147	74.996	44.126	14.306	1.00	36.03
1983	OE1	GLU		147	74.447	44.128	13.102	1.00	38.00
1984	OE2	GLU		147	74.447	44.556	15.102	1.00	37.12
1985	C	GLU		147	78.224	45.857	16.976	1.00	28.68
1986	0	GLU		147	79.335	46.129	16.528	1.00	28.50
1987	N	VAL		148	77.599	46.613	17.879	1.00	26.68
1989	CA	VAL		148	78.056	47.949	18.205	1.00	25.01
1991	СВ	VAL		148	76.886	48.966	18.244	1.00	
1993	CG1	VAL		148	77.404	50.369	18.438	1.00	
1997	CG2	VAL		148	76.049	48.887	16.950	1.00	24.80
2001	C	VAL		148	78.819	47.927	19.526	1.00	23.84
2002	ō	VAL		148	78.271	47.605	20.585	1.00	
2003	N	SER		149	80.098	48.254	19.440	1.00	
2005	CA	SER		149	80.952	48.338	20.613	1.00	
2007	СВ	SER		149	82.404	48.597	20.186	1.00	
2010	OG	SER		149	82.568	49.915	19.707	1.00	21.57
2012	С	SER	Α	149	80.458	49.448	21.539	1.00	23.11
2013	0	SER	Α	149	79.794	50.402	21.099	1.00	21.95
2014	N	ASP	Α	150	80.777	49.313	22.817	1.00	23.66
2016	CA	ASP	Α	150	80.499	50.348	23.801		24.49
2018	CB	ASP	Α	150	81.010	49.930	25.172	1.00	25.14
2021	CG	ASP	Α	150	80.256	48.733	25.735	1.00	27.65
2022	OD1	ASP	Α	150	80.719	48.186	26.762	1.00	31.30
2023	OD2	ASP	Α	150	79.201	48.281	25.225	1.00	27.89
2024	С	ASP	A	150	81.115	51.680	23.394	1.00	24.45
2025	0	ASP	Α	150	80.499	52.725	23.568	1.00	23.41
2026	N	ARG	A	151	82.319	51.639	22.827		24.28
2028	CA	ARG		151	82.973	52.844	22.355		24.79
2030	CB	ARG		151	84.352	52.508	21.759	1.00	26.00
2033	CG	ARG		151	85.134	53.699	21.268		28.93
2036	CD	ARG		151	85.432	54.712	22.350		34.80
2039	NE	ARG		151	84.576	55.893	22.233		38.89
2041	CZ	ARG		151	84.277	56.711	23.229		42.07
2042	NH1	ARG	Α	151	83.494	57.756	22.989	1.00	43.97

FIGURE 3 (Cont.) AU

Α	В	С	D	E	F	G	Н	I	J
2045	NH2	ARG		151	84.754	56.502	24.462	1.00	42.69
2048	С	ARG		151	82.119	53.534	21.303		23.63
2049	0	ARG		151	81.949	54.749	21.330	1.00	22.68
2050	N	ASP		152	81.578	52.751	20.377	1.00	22.64
2052	CA	ASP		152	80.765	53.305	19.316	1.00	22.05
2054	CB		Α	152	80.695	52.351	18.126	1.00	22.68
2057	CG	ASP		152	82.013	52.303	17.348	1.00	24.58
2058	OD1	ASP		152	82.780	53.285	17.412	1.00	24.51
2059	OD2		Α	152	82.369	51.328	16.654	1.00	27.53
2060	C	ASP		152	79.380	53.730	19.832	1.00	20.89
2061	0	ASP		152	78.829	54.703	19.348	1.00	19.41
2062	N	ARG		153	78.855	53.043	20.844	1.00	19.83
2064	CA	ARG		153	77.577	53.435	21.459	1.00	18.66
2066	CB	ARG		153	77.116	52.390	22.450	1.00	18.96
2069	CG	ARG		153	75.734	52.644	23.008	1.00	18.87
2072	CD	ARG		153	75.377	51.687	24.112	1.00	19.73
2075	NE	ARG		153	75.180	50.322	23.630	1.00	20.07
2077	CZ	ARG		153	73.991	49.773	23.369	1.00	22.06
2078	NH1	ARG		153	73.929	48.516	22.949	1.00	20.83
2081	NH2	ARG		153	72.862	50.466	23.521	1.00	23.23
2084	C	ARG		153	77.724	54.771	22.171	1.00	18.18
2085	0	ARG		153	76.842	55.612	22.081	1.00	17.20
2086	N	ILE		154	78.847	54.959	22.869	1.00	17.73
2088	CA	ILE		154	79.141	56.223	23.542	1.00	18.41
2090	CB	ILE		154	80.414	56.100	24.449	1.00	18.14
2092	CG1	ILE		154	80.092	55.249	25.684	1.00	19.24
2095	CD1	ILE		154	81.307	54.703	26.408	1.00	20.01
2099	CG2		A	154	80.932	57.468	24.875	1.00	19.53
2103	C	ILE		154	79.277	57.343	22.505	1.00	17.74
2104	0	ILE		154	78.757	58.424	22.698	1.00	18.17
2105	N CA	SER		155	79.934	57.063	21.388	1.00	18.18
2107	CA	SER		155	80.095	58.043	20.323	1.00	18.52
2109 2112	CB OG	SER SER		155	81.020	57.511	19.236	1.00	18.63
2112	C			155	82.330	57.395	19.748	1.00	18.50
2114	0	SER SER		155	78.744	58.437	19.718	1.00	19.05
2116	N	MET		155	78.538	59.594	19.368	1.00	19.13
			_	156	77.836	57.476	19.618	1.00	19.12
2118 2120	CA CB	MET MET		156 156	76.482 75.674	57.743	19.135		19.40
2123	CG	MET		156	76.083	56.461	19.063 17.948		19.56 22.23
2126	SD	MET		156	74.922	55.564 54.182			28.16
2127	CE	MET		156	75.814	53.241	17.803	1.00	
2131	C	MET		156	75.746	58.693	16.666 20.039	1.00	
2132	0	MET		156	75.740	59.609	19.567	1.00	18.61 18.79
2133	N	ILE		157	75.826	58.439	21.342	1.00	
2135	CA	ILE		157	75.826	59.281	22.349	1.00	18.55 17.91
2137	CB	ILE		157	75.194	58.649	23.752	1.00	17.84
2139	CG1	ILE		157	74.511	57.360	23.732	1.00	18.27
2142	CD1	ILE		157	74.814	56.495	25.017	1.00	18.88
2146	CG2	ILE		157	74.941	59.646	24.845		17.97
2150	C	ILE		157	75.804	60.685	22.313	1.00	17.61
2151	Ö	ILE		157	75.087	61.683	22.308	1.00	
	_							• •	

FIGURE 3 (Cont.) AV

2152 N	Α	В	С	D	E	F	G	H	I	J
2154 CA SER A 158 77.856 62.012 22.247 1.00 17.24 2156 CB SER A 158 79.372 61.759 22.292 1.00 17.57 2161 C SER A 158 77.487 62.988 21.093 1.00 17.58 2162 O SER A 158 77.487 62.819 21.093 1.00 17.58 2163 N GLU A 159 77.408 62.163 18.986 1.00 18.38 2167 CB GLU A 159 77.042 61.904 17.409 1.00 19.18 2170 CG GLU A 159 76.518 62.361 16.145 1.00 20.75 2174 OE1 GLU A 159 76.518 62.361 16.049 1.00 20.37 2175 OE2 GLU A 159 75.591 <td>2152</td> <td>3.7</td> <td>O.D.D.</td> <td></td> <td>150</td> <td>DD 136</td> <td>60 540</td> <td></td> <td></td> <td></td>	2152	3.7	O.D.D.		150	DD 136	60 540			
2156 CB SER A 158 79.372 61.759 22.292 1.00 16.92 2151 C SER A 158 80.087 62.908 21.936 1.00 16.92 2161 C SER A 158 77.466 62.903 21.007 1.00 17.17 2163 N GLU A 159 77.404 62.2833 18.616 1.00 18.63 2165 CA GLU A 159 77.042 62.933 18.616 1.00 19.18 2170 CG GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.518 62.361 16.145 1.00 20.77 2175 OE2 GLU A 159 76.531 <td></td>										
2159 OG SER A 158 80.087 62.908 21.936 1.00 16.92 2161 C SER A 158 77.487 62.819 21.007 1.00 17.58 2163 O SER A 158 77.408 62.163 19.856 1.00 18.38 2165 CA GLU A 159 77.042 62.833 18.616 1.00 10.63 2167 CB GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.518 62.361 16.145 1.00 20.77 2174 OEI GLU A 159 78.105 64.141 16.00 20.445 2175 OEZ GLU A 159 75.531 64.455 18.224 1.00 18.98 2176 C GLU A 159 75.531 64.455 18.224 1.00 18.98 2177 O GLU A </td <td></td>										
2161 C SER A 158 77.487 62.819 21.007 1.00 17.58 2163 N GLU A 159 77.408 62.163 19.856 1.00 18.63 2165 CA GLU A 159 77.042 62.833 18.616 1.00 18.63 2167 CG GLU A 159 77.042 62.833 18.616 1.00 19.18 2170 CG GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.979 63.726 15.666 1.00 23.75 2175 OE2 GLU A 159 76.233 64.384 14.918 1.00 26.52 2175 OE2 GLU A 159 75.592 63.324 18.648 1.00 18.93 2175 OE2 GLU A 159 75.511 64.455 18.224 1.00 18.93 2176 C GLU A 160 73.274 62.921 19.169 1.00 19.20										
2162 O SER A 158 77.266 64.003 21.093 1.00 17.17 2163 N GLU A 159 77.408 62.163 19.956 1.00 18.38 2167 CB GLU A 159 77.042 62.833 18.616 1.00 18.38 2167 CB GLU A 159 77.242 61.904 17.409 1.00 19.18 2170 CG GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.979 63.726 15.666 1.00 24.45 2175 CEZ GLU A 159 76.979 63.726 18.648 1.00 26.52 2176 C GLU A 159 75.592 63.324 18.648 1.00 18.41 2177 O GLU A 159 75.511 64.455 18.224 1.00 18.41 2177 O GLU A 160 74.671 62.489 19.122 1.00 18.5 2180 C LEU A 160 73.274 62.213 19.337 1.00 20.										
2165 CA GLU A 159 77.408 62.163 19.856 1.00 18.38 2167 CB GLU A 159 77.042 62.833 18.616 1.00 18.63 2167 CB GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.518 62.361 16.145 1.00 20.77 2174 OE1 GLU A 159 76.579 63.726 15.666 1.00 23.75 2175 OE2 GLU A 159 75.592 63.324 18.648 1.00 18.90 2177 O GLU A 159 75.511 64.455 18.224 1.00 18.90 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.98 2180 CB LEU A 160 73.274 62.921 19.169 1.00 18.98 2185 C LEU A 160 70.528 62.479 17.890 1.00 20.04 <										
2165 CA GLU A 159 77.042 62.833 18.616 1.00 18.63 2167 CB GLU A 159 77.242 61.904 17.409 1.00 19.18 2173 CD GLU A 159 76.518 62.361 16.145 1.00 23.75 2174 OEI GLU A 159 76.979 63.726 15.666 1.00 23.75 2175 OE2 GLU A 159 76.979 63.726 15.666 1.00 24.45 2175 OE2 GLU A 159 75.592 63.324 18.648 1.00 18.90 2177 O GLU A 150 75.311 64.455 18.224 1.00 18.91 2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.92 2181 CB LEU A 160 70.845 62.123 19.337 1.00 20.04 2185 CEU A										
2167										
2170 CG GLU A 159 76.518 62.361 16.145 1.00 20.77 2173 CD GLU A 159 76.979 63.726 15.666 1.00 23.75 2175 OE2 GLU A 159 76.233 64.384 14.918 1.00 24.45 2176 CE GLU A 159 75.592 63.324 18.648 1.00 18.90 2177 O GLU A 159 75.592 63.324 18.648 1.00 18.90 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.98 2180 CA LEU A 160 73.274 62.921 19.169 1.00 19.20 2185 CG LEU A 160 70.528 62.479 17.890 1.00 20.03 2187 CD1 LEU A 160 70.015 60.977 19.795 1.00 20.04 2195 C LEU A										
2173 CD GLU A 159 76.979 63.726 15.666 1.00 23.75 2174 OE1 GLU A 159 78.105 64.141 16.022 1.00 24.45 2175 OE2 GLU A 159 76.233 64.384 14.918 1.00 26.52 2176 C GLU A 159 75.511 64.455 18.224 1.00 18.41 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.93 2180 CA LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CDI LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.528 66.2479 17.890 1.00 20.02 2195 C LEU A 160 70.15 60.977 19.795 1.00 21.02 2195 C<							61.904	17.409	1.00	19.18
2174 OE1 GLU A 159 78.105 64.141 16.022 1.00 24.45 2175 OE2 GLU A 159 76.233 64.384 14.918 1.00 26.52 2177 O GLU A 159 75.592 63.324 18.648 1.00 18.90 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.15 2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.15 2185 CB LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.03 2195 C LEU A 160 73.319 64.115 20.113 1.00 21.02 2195 C LEU A 160 73.834 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>16.145</td> <td>1.00</td> <td>20.77</td>								16.145	1.00	20.77
2175 OE2 GLU A 159 76.233 64.384 14.918 1.00 26.52 2176 C GLU A 159 75.592 63.324 18.648 1.00 18.90 2177 O GLU A 159 75.511 64.455 18.224 1.00 18.41 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.15 2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.98 2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.119 64.115 20.113 1.00 21.02 2197 N ALA A 161 73.814 65.062 22.208 1.00 20.64 2207 CB ALA A 161 73.814 65.162 22.208 1.00 20.64 <td></td> <td></td> <td></td> <td></td> <td></td> <td>76.979</td> <td>63.726</td> <td>15.666</td> <td>1.00</td> <td>23.75</td>						76.979	63.726	15.666	1.00	23.75
2176 C GLU A 159 75.592 63.324 18.648 1.00 18.90 2177 O GLU A 159 75.311 64.455 18.224 1.00 18.41 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.98 2185 CB LEU A 160 73.274 62.921 19.169 1.00 18.98 2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.04 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.15 60.977 19.795 1.00 20.04 2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 C LEU A 160 73.814 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.814 65.162 22.208 1.00 20.54		OE1	GLU	Α	159	78.105	64.141	16.022	1.00	24.45
2177 O GLU A 159 75.311 64.455 18.224 1.00 18.41 2178 N LEU A 160 74.671 62.489 19.122 1.00 18.15 2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.98 2185 CB LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.319 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA 161 73.832 64.078 21.234 1.00 19.99 2199 CA	2175	OE2	GLU	Α	159	76.233		14.918	1.00	26.52
2178 N LEU A 160 74.671 62.489 19.122 1.00 18.15 2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.98 2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 73.832 64.078 21.234 1.00 19.39 2197 N ALA A 161 73.832 64.078 21.234 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.54 2205 C <td>2176</td> <td>C</td> <td></td> <td></td> <td>159</td> <td>75.592</td> <td>63.324</td> <td>18.648</td> <td>1.00</td> <td>18.90</td>	2176	C			159	75.592	63.324	18.648	1.00	18.90
2180 CA LEU A 160 73.274 62.921 19.169 1.00 18.98 2182 CB LEU A 160 72.333 61.801 19.559 1.00 19.20 2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2201 CB ALA A 161 73.690 67.496 21.678 1.00 20.84 2207 N <td></td> <td>0</td> <td>GLU</td> <td>Α</td> <td>159</td> <td>75.311</td> <td>64.455</td> <td>18.224</td> <td>1.00</td> <td>18.41</td>		0	GLU	Α	159	75.311	64.455	18.224	1.00	18.41
2182 CB LEU A 160 72.333 61.801 19.559 1.00 19.20 2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA 161 73.814 65.162 22.208 1.00 20.76 2201 CB ALA 161 74.362 66.466 21.621 1.00 20.84 2205 C ALA 161 74.362 66.466 21.678 1.00 21.05 2207 N	2178	N	LEU	Α	160	74.671	62.489	19.122	1.00	18.15
2185 CG LEU A 160 70.845 62.123 19.337 1.00 20.03 2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2195 C LEU A 160 70.015 60.977 19.795 1.00 21.02 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2201 CB ALA A 161 74.362 66.466 21.621 1.00 20.76 2205 C ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.546 66.431 21.027 1.00 21.51 2209 CA	2180	CA	LEU	Α	160	73.274	62.921	19.169	1.00	18.98
2187 CD1 LEU A 160 70.528 62.479 17.890 1.00 20.04 2191 CD2 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 72.388 65.058 19.808 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA 161 74.362 66.466 21.678 1.00 20.84 2206 O ALA 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 77.614 67.492 20.063	2182	CB	LEU	Α	160	72.333	61.801	19.559	1.00	19.20
2191 CD2 LEU A 160 70.015 60.977 19.795 1.00 21.02 2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.832 64.078 21.234 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.621 1.00 20.76 2205 C ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.461 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2207 CA SER A 162 77.614 67.492 20.063 1.00 22.37	2185	CG	LEU	Α	160	70.845	62.123	19.337	1.00	20.03
2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.832 64.078 21.234 1.00 19.92 2199 CA ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.621 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 77.614 67.492 20.63 1.00 22.08 2214 OG SER A 162 77.809 66.365 19.248 1.00 22.18 2216 C	2187	CD1	LEU	Α	160	70.528	62.479	17.890	1.00	20.04
2195 C LEU A 160 73.119 64.115 20.113 1.00 19.39 2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.832 64.078 21.234 1.00 19.92 2199 CA ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.621 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 77.614 67.492 20.63 1.00 22.08 2214 OG SER A 162 77.809 66.365 19.248 1.00 22.18 2216 C	2191	CD2	LEU	Α	160	70.015	60.977	19.795	1.00	21.02
2196 O LEU A 160 72.388 65.058 19.808 1.00 19.39 2197 N ALA A 161 73.832 64.078 21.234 1.00 19.92 2199 CA ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.621 1.00 20.88 2206 O ALA A 161 73.690 67.496 21.6278 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.55 2209 CA SER A 162 77.614 67.492 20.063 1.00 22.08 2211 CB SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C	2195	C	LEU	Α	160		64.115		1.00	
2197 N ALA A 161 73.832 64.078 21.234 1.00 19.92 2199 CA ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.621 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 77.614 67.492 20.063 1.00 22.37 2211 CB SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N	2196	0	LEU	A	160	72.388	65.058	19.808	1.00	
2199 CA ALA A 161 73.814 65.162 22.208 1.00 20.54 2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.678 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 76.138 67.660 20.486 1.00 22.08 2214 OG SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 20.07 2218 N	2197	N	ALA	Α	161	73.832	64.078			19.92
2201 CB ALA A 161 74.591 64.764 23.463 1.00 20.76 2205 C ALA A 161 74.362 66.466 21.678 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2221 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2225 CB	2199	CA	ALA	Α	161	73.814				20.54
2205 C ALA A 161 74.362 66.466 21.621 1.00 20.84 2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 76.138 67.660 20.486 1.00 22.08 2211 CB SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2222 CB ALA A 163 73.906 67.716 17.379 1.00 20.07 2224 CB	2201	CB	ALA	Α	161	74.591	64.764	23.463		
2206 O ALA A 161 73.690 67.496 21.678 1.00 21.05 2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 76.138 67.660 20.486 1.00 22.08 2211 CB SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.732 66.523 16.438 1.00 20.07 2222 CB ALA A 163 71.937 69.041 17.026 1.00 18.96	2205	С	ALA	Α	161	74.362	66.466			20.84
2207 N SER A 162 75.554 66.431 21.027 1.00 21.51 2209 CA SER A 162 76.138 67.660 20.486 1.00 22.08 2211 CB SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 71.937 69.041 17.026 1.00 18.96 2227 O	2206	0	ALA	Α	161	73.690	67.496		1.00	
2209 CA SER A 162 76.138 67.660 20.486 1.00 22.08 2211 CB SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2230 CA	2207	N	SER	Α	162	75.554	66.431			
2211 CB SER A 162 77.614 67.492 20.063 1.00 22.37 2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 20.43 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.07 2220 CA ALA A 163 73.732 66.523 16.438 1.00 20.07 2222 CB ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB	2209	CA	SER	Α	162	76.138	67.660		1.00	
2214 OG SER A 162 77.809 66.365 19.248 1.00 24.18 2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 71.937 69.041 17.026 1.00 18.96 2227 O ALA A 163 71.937 69.041 17.026 1.00 19.77 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 233 CB	2211	CB	SER	Α	162			20.063		
2216 C SER A 162 75.286 68.207 19.336 1.00 21.42 2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.71 2330 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2325 OG	2214	OG	SER	Α	162	77.809	66.365	19.248	1.00	24.18
2217 O SER A 162 75.142 69.415 19.197 1.00 21.65 2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77	2216	С	SER	Α	162		68.207	19.336		
2218 N ALA A 163 74.700 67.316 18.539 1.00 20.43 2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10			SER	Α		75.142				
2220 CA ALA A 163 73.906 67.716 17.379 1.00 20.07 2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655		N	ALA	Α						
2222 CB ALA A 163 73.732 66.523 16.438 1.00 20.07 2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY	2220	CA	ALA	Α		73.906				
2226 C ALA A 163 72.537 68.265 17.768 1.00 19.77 2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.71 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 <td></td> <td>СB</td> <td>ALA</td> <td>Α</td> <td>163</td> <td></td> <td></td> <td></td> <td></td> <td></td>		СB	ALA	Α	163					
2227 O ALA A 163 71.937 69.041 17.026 1.00 18.96 2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.86			ALA	Α						
2228 N SER A 164 72.026 67.836 18.922 1.00 19.92 2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86										
2230 CA SER A 164 70.677 68.207 19.366 1.00 19.71 2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84										
2232 CB SER A 164 70.061 67.027 20.112 1.00 20.08 2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA		CA								
2235 OG SER A 164 70.098 65.862 19.285 1.00 21.77 2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71	2232									
2237 C SER A 164 70.655 69.452 20.246 1.00 20.10 2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71										
2238 O SER A 164 69.661 70.210 20.271 1.00 18.98 2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71										
2239 N GLY A 165 71.757 69.676 20.958 1.00 19.76 2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71	2238	0	SER	Α						
2241 CA GLY A 165 71.846 70.733 21.939 1.00 20.35 2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71		N								
2244 C GLY A 165 72.244 72.081 21.365 1.00 20.96 2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71										
2245 O GLY A 165 71.982 72.393 20.203 1.00 20.86 2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71										
2246 N ILE A 166 72.900 72.879 22.200 1.00 21.84 2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71										
2248 CA ILE A 166 73.170 74.280 21.914 1.00 22.71	2246									
	2250	СВ	ILE	Α						

FIGURE 3 (Cont.) AW

A	В	С	D	E	F	G	Н	I	J
2252	CG1	ILE	Α	166	73.194	76.437	23.239	1.00	23.87
2255	CD1	ILE		166	71.710	76.610	23.444		23.14
2259	CG2	ILE		166	75.109	74.770	23.489		25.44
2263	C	ILE		166	74.197	74.443	20.769		22.75
2264	Ö	ILE		166	74.206	75.456	20.763	1.00	
2265	N	ALA		167	75.027	73.430	20.572		22.36
2267	CA	ALA		167	75.954	73.422	19.451		
2269	CB	ALA		167			19.770		22.62
					77.109	72.455			22.85
2273 2274	C	ALA		167	75.285	72.916	18.152		22.34
	O N	ALA		167	75.905	72.963	17.111		22.65
2275	N	GLY		168	74.028	72.488	18.212	1.00	
2277	CA	GLY		168	73.304	72.064	17.022	1.00	21.12
2280	C	GLY		168	71.883	72.588	16.982		20.68
2281	0	GLY		168	71.665	73.785	16.956	1.00	19.79
2282	N	MET		169	70.914	71.682	17.005		20.95
2284	CA	MET		169	69.501	72.019	16.812	1.00	
2286	СВ	MET		169	68.655	70.757	16.927	1.00	
2289	CG	MET		169	67.183	70.922	16.531	1.00	
2292	SD	MET	Α	169	66.208	71.479	17.897	1.00	28.34
2293	CE	MET	Α	169	66.254	69.967	19.003	1.00	25.97
2297	С		Α	169	68.952	73.140	17.721	1.00	20.52
2298	0	MET		169	68.310	74.072	17.224	1.00	19.77
2299	N	CYS	Α	170	69.200	73.059	19.028	1.00	20.60
2301	CA	CYS	Α	170	68.689	74.061	19.977	1.00	20.42
2303	CB I	BCYS	Α	170	68.958	73.590	21.405	0.35	20.62
2304		ACYS		170	68.958	73.668	21.427	0.65	20.89
2309	SG 1	BCYS	Α	170	67.803	74.234	22.609	0.35	20.91
2310	SG 2	ACYS	Α	170	67.804	72.489	22.098	0.65	22.71
2311	C	CYS	A	170	69.332	75.426	19.744	1.00	20.33
2312	0	CYS	Α	170	68.665	76.459	19.811	1.00	18.74
2313	N	GLY	Α	171	70.650	75.414	19.539	1.00	20.11
2315	CA	GLY	Α	171	71.384	76.605	19.172	1.00	20.26
2318	C	GLY	Α	171	70.807	77.252	17.932	1.00	20.35
2319	0	GLY	Α	171	70.645	78.473	17.877	1.00	19.82
2320	N	GLY	Α	172	70.470	76.425	16.948	1.00	20.20
2322	CA	GLY	Α	172	69.875	76.891	15.715	1.00	20.43
2325	C	GLY	Α	172	68.484	77.441	15.920	1.00	20.51
2326	0	GLY	Α	172	68.117	78.435	15.303	1.00	20.93
2327	N	GLN	Α	173	67.716	76.816	16.800	1.00	20.70
2329	CA	GLN	Α	173	66.397	77.327	17.168		21.15
2331	CB	GLN	Α	173	65.684	76.383	18.149		21.47
2334	CG	GLN	Α	173	65.165	75.072	17.546		21.62
2337	CD	GLN	Α	173	64.102	75.279	16.494		22.97
2338	OE1	GLN	Α	173	64.417	75.656	15.362		27.11
2339	NE2			173	62.845	75.031	16.850		22.24
2342	С	GLN		173	66.514	78.725	17.794		21.59
2343	0	GLN		173	65.695	79.609	17.513		22.14
2344	N	ALA		174	67.532	78.931	18.622		21.59
2346	CA	ALA		174	67.766	80.245	19.230		21.99
2348	CB	ALA		174	68.847	80.166	20.296		22.20
2352	С	ALA		174	68.152	81.269	18.164		22.07
2353	0	ALA		174	67.683	82.380	18.206		21.87

FIGURE 3 (Cont.) AX

A	В	С	D	E	F	G	H	I	J
2354	N	LEU	Δ	175	69.001	80.885	17.212	1 00	22.13
2356	CA	LEU		175	69.369	81.776	16.106		23.00
2358	СВ	LEU		175	70.449	81.144	15.233	1.00	
2361	CG	LEU		175	71.824	80.871	15.840	1.00	22.66
2363	CD1	LEU		175	72.668	80.085	14.817	1.00	24.29
2367	CD2	LEU		175	72.522	82.155	16.235	1.00	22.45
2371	C	LEU		175	68.163	82.119	15.240	1.00	23.28
2372	Ö	LEU		175	68.003	83.265	14.805	1.00	23.62
2372	N		A	176	67.314	81.123	15.002	1.00	
2375	CA	ASP	A	176	66.112	81.280	14.197	1.00	24.49
2377	CB	ASP	Α	176	65.382	79.934	14.080	1.00	24.90
2380	CG		A	176	64.004	80.064	13.491	1.00	25.57
2381			A	176	63.830	79.750	12.287	1.00	28.64
2382	OD2	ASP		176	63.023	80.441	14.162	1.00	
2383	C	ASP		176	65.187	82.320	14.102	1.00	24.97
2384	Ö	ASP		176	64.683	83.222	14.178	1.00	24.47
2385	N	LEU		177	64.974	82.168	16.138	1.00	25.23
2387	CA	LEU		177	64.127	83.083	16.905	1.00	26.68
2389	CB	LEU		177	63.977	82.575	18.343	1.00	26.78
2392	CG	LEU		177	62.658	81.902	18.734	1.00	28.22
2394	CD1	LEU		177	62.016	81.077	17.633	1.00	29.14
2398	CD2	LEU		177	62.892	81.055	19.970	1.00	29.13
2402	C	LEU		177	64.686	84.512	16.914	1.00	26.76
2403	ō	LEU		177	63.936	85.474	16.784	1.00	26.89
2404	N	ASP		178	66.002	84.640	17.050	1.00	27.40
2406	CA	ASP		178	66.636	85.952	17.078	1.00	28.30
2408	СВ		Α	178	68.107	85.827	17.459	1.00	28.53
2411	CG	ASP	Α	178	68.753	87.176	17.720	1.00	31.35
2412	OD1	ASP	Α	178	69.682	87.571	16.965	1.00	33.39
2413	OD2	ASP	Α	178	68.389	87.907	18.667	1.00	33.95
2414	С	ASP	Α	178	66.513	86.681	15.734	1.00	28.03
2415	0	ASP	Α	178	66.398	87.907	15.689	1.00	27.69
2416	N	ALA	Α	179	66.525	85.915	14.648	1.00	27.46
2418	CA	ALA	Α	179	66.499	86.467	13.300	1.00	27.69
2420	CB	ALA	Α	179	67.174	85.479	12.330	1.00	27.70
2424	С	ALA	Α	179	65.089	86.843	12.796	1.00	27.58
2425	0	ALA		179	64.946	87.351	11.683	1.00	27.80
2426	N	GLU		180	64.057	86.590	13.596		27.88
2428	CA	GLU		180	62.702	87.040	13.277		28.36
2430	CB	GLU		180	61.710	86.633	14.367		28.57
2433	CG	GLU		180	61.415	85.151	14.422		29.97
2436	CD	GLU		180	60.434	84.780	15.517		32.47
2437		GLU		180	60.070	85.661	16.338		34.93
2438		GLU		180	60.026	83.598	15.558		32.41
2439	C	GLU		180	62.695	88.560	13.162		28.40
2440	O N	GLU		180	63.140	89.252	14.075		27.70
2441 2443	N CA	GLY		181	62.227	89.057	12.020	1.00	
2443	CA C	GLY GLY		181 181	62.105 63.391	90.477 91.173	11.766 11.391	1.00	29.05 29.41
2446	0	GLY		181	63.379	92.382	11.391		30.34
2447	И	LYS		182	64.501	90.437	11.129		29.52
2450	CA	LYS		182	65.818	91.032	11.137		29.52
			••		00.010		,_,	1.00	22.20

FIGURE 3 (Cont.) AY

2452 CB LYS A 182 66.807 90.510 12.175 1.00 30.25 2458 CD LYS A 182 66.415 90.819 13.604 1.00 31.19 2461 CE LYS A 182 67.168 90.894 16.009 1.00 34.43 2468 C LYS A 182 65.969 90.778 16.00 29.31 2469 O LYS A 182 66.375 90.797 7.30 1.00 29.31 2470 N HIS A 183 65.725 89.944 8.947 1.00 29.18 2472 CA HIS A 183 66.575 90.895 6.686 1.00 29.50 2477 CB HIS A 183 66.297 91.086 6.806 1.00 29.52 2477 CB HIS A 183 67.982 90.944	Α	В	C	D	E	F	G	Н	I	J
2455 CG LYS 182 66.415 90.819 13.604 1.00 31.19 2456 CE LYS A 182 67.528 90.474 14.569 1.00 33.42 2461 CE LYS A 182 67.168 90.894 16.009 1.00 34.43 2468 C LYS A 182 65.969 90.178 16.544 1.00 36.01 2470 N HIS A 182 66.375 90.797 9.730 1.00 29.51 2472 CA HIS A 183 66.798 89.736 7.546 1.00 29.54 2474 CB HIS A 183 65.574 90.895 6.688 1.00 29.54 2478 NDI HIS A 183 63.217 90.679 5.835 1.00 29.03 2478 NDI HIS A 183 63.217 90.679<	2452	СВ	LYS	Α	182	66.807	90.510	12.175	1.00	30.25
2456 CE LYS 182 67.528 90.474 14.569 1.00 33.42 2461 CE LYS A 182 67.168 90.894 16.009 1.00 34.43 2468 NZ LYS A 182 65.969 90.178 16.544 1.00 36.01 2469 O LYS A 182 66.375 90.797 9.730 1.00 29.18 2470 N HIS A 183 65.725 89.944 8.947 1.00 29.53 2474 CB HIS A 183 65.574 89.944 8.947 1.00 29.50 2474 CB HIS A 183 66.099 91.086 6.888 1.00 29.50 2477 CG HIS A 183 63.217 90.679 5.835 1.00 29.33 2480 NE2 HIS A 183 63.217 90.679 <td></td>										
2461 CE LYS A 182 65.969 90.178 16.009 1.00 34.43 2468 C LYS A 182 65.969 90.178 16.544 1.00 36.01 2469 O LYS A 182 66.375 90.797 9.730 1.00 29.31 2470 N HIS A 183 65.725 89.944 8.947 1.00 29.50 2477 CB HIS A 183 66.098 99.895 6.688 1.00 29.50 2477 CG HIS A 183 66.099 91.086 6.806 1.00 29.50 2478 NDI HIS A 183 63.217 90.679 5.835 1.00 29.04 2488 CE1 HIS A 183 63.217 90.944 6.226 1.00 30.87 2484 CD2 HIS A 183 67.598										
2464 NZ LYS A 182 66.375 90.178 16.544 1.00 36.01 2469 O LYS A 182 66.375 90.737 9.730 1.00 29.61 2470 N HIS A 183 65.725 89.944 8.947 1.00 29.18 2474 CA HIS A 183 66.098 89.736 7.546 1.00 29.54 2477 CG HIS A 183 66.098 89.736 6.586 1.00 29.04 2478 BHIS A 183 66.572 90.679 5.835 1.00 29.04 2480 CEI HIS A 183 63.217 90.679 5.835 1.00 29.33 2480 NE HIS A 183 63.346 91.580 7.816 1.00 30.77 2486 C HIS A 183 66.261 90.375										
2468 C LYS A 182 66.375 90.797 9.730 1.00 29.61 2469 O LYS A 182 67.389 91.383 9.367 1.00 29.31 2472 CA HIS A 183 66.098 89.736 7.546 1.00 29.54 2474 CB HIS A 183 66.098 89.736 7.546 1.00 29.50 2477 CG HIS A 183 66.098 89.736 7.546 1.00 29.50 2477 GG HIS 183 66.096 6.606 6.00 1.00 29.33 2480 NE2 HIS 183 61.982 90.944 6.226 1.00 30.87 2482 NE2 HIS 183 67.598 89.588 7.410 1.00 29.52 2487 O HIS 183 68.261 90.39 6.732 1.00 29.81										
2469 O LYS A 182 67.389 91.383 9.367 1.00 29.31 2470 N HIS A 183 65.725 89.944 8.947 1.00 29.51 2474 CB HIS A 183 66.098 89.736 6.688 1.00 29.50 2477 CG HIS A 183 64.099 91.086 6.806 1.00 29.04 2478 NDI HIS A 183 64.099 91.086 6.806 1.00 29.33 2488 NDI HIS A 183 63.217 90.679 5.835 1.00 29.33 2486 CEI HIS A 183 62.033 91.486 7.429 1.00 30.69 2486 C HIS A 183 68.261 90.375 6.732 1.00 29.52 2490 CA VAL A 184 69.566										
2470 N HIS A 183 65.725 89.944 8.947 1.00 29.18 2472 CA HIS A 183 66.098 89.736 7.546 1.00 29.50 2477 CG HIS A 183 64.099 91.086 6.806 1.00 29.04 2478 NDI HIS A 183 63.217 90.679 5.835 1.00 29.33 2480 CEI HIS A 183 62.033 91.486 7.429 1.00 30.67 2486 NEZ HIS A 183 67.598 89.588 7.410 1.00 29.52 2486 C HIS A 183 66.261 90.375 6.732 1.00 29.52 2487 O HIS A 184 69.580 88.461 8.215 1.00 29.52 2492 CB VAL A 184 69.580	2469	0	LYS	Α						
2472 CA HIS A 183 66.098 89.736 7.546 1.00 29.54 2477 CB HIS A 183 65.574 90.895 6.688 1.00 29.04 2478 ND1 HIS A 183 64.099 91.086 6.806 1.00 29.03 2480 CEI HIS A 183 61.982 90.944 6.226 1.00 30.87 2484 CE2 HIS A 183 62.033 91.486 7.429 1.00 30.67 2486 CD HIS A 183 63.346 91.580 7.816 1.00 29.52 2487 O HIS A 183 66.261 90.375 6.732 1.00 29.52 2488 N VAL A 184 69.580 88.461 8.215 1.00 29.52 2490 CB VAL A 184 69.580 88.461 8.215 1.00 29.52 2494 CGI		N	HIS	Α						
2474 CB HIS A 183 65.574 90.895 6.688 1.00 29.50 2477 CG HIS A 183 64.099 91.086 6.806 1.00 29.04 2478 ND1 HIS A 183 63.217 90.679 5.835 1.00 29.33 2480 CE1 HIS A 183 62.033 91.486 7.429 1.00 30.87 2482 NE2 HIS A 183 62.033 91.486 7.429 1.00 30.77 2484 CD2 HIS A 183 63.346 91.580 7.816 1.00 29.56 2486 C HIS A 183 67.598 89.588 7.410 1.00 29.56 2487 O HIS A 183 68.261 90.375 6.732 1.00 29.82 2488 N VAL A 184 68.136 88.569 80.667 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.52 2490 CA VAL A 184 69.976 87.488 9.352 1.00 29.40 2492 CB VAL A 184 69.976 87.488 9.352 1.00 29.32 2498 CG2 VAL A 184 69.310 87.904 10.659 1.00 29.32 2498 CG2 VAL A 184 69.310 87.904 10.659 1.00 29.32 2498 CG2 VAL A 184 69.586 87.448 6.037 1.00 29.32 2498 CG2 VAL A 184 69.586 87.448 6.037 1.00 29.64 2502 C VAL A 184 70.233 88.072 6.886 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.72 2505 CA PRO A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 72.217 88.446 5.458 1.00 29.72 2510 CG PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.369 89.766 6.777 1.00 30.18 2513 CD PRO A 185 73.389 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.217 85.896 6.224 1.00 29.95 2517 O PRO A 185 72.357 89.168 7.653 1.00 29.95 2517 O PRO A 185 72.348 86.679 5.266 1.00 29.95 2517 O PRO A 185 72.448 86.659 5.266 1.00 29.95 2518 N LEU A 186 73.369 89.168 6.224 1.00 30.74 2520 CB LEU A 186 73.604 83.417 1.548 1.00 30.90 2525 CG LEU A 186 73.604 83.417 1.548 1.00 30.74 2520 CB LEU A 186 73.604 83.417 1.548 1.00 30.74 2531 CD LEU A 186 73.472 82.997 5.093 1.00 30.74 2533 N ASP A 187 77.078 84.667 6.143 1.00 30.74 2534 CB ASP A 187 77.079 86.128 6.641 1.00 37.70 2546 CD ASP A 187 75.951 83.903 5.945 1.00 31.77 2541 CB ASP A 187 75.951 83.903 5.945 1.00 31.77 2546 CD ASP A 187 75.951 83.903 5.945 1.00 31.77 2547 C ASP A 187 75.951 86.866 6.881 1.00 30.74 2549 N ALA A 188 73.761 84.297 9.082 1.00 30.74 2540 CD ASP A 187 75.951 86.866 6.881 1.00 30.74 2549 N ALA A 188 73.761 84.297 9.082 1.00 30.74 2540 C ASP A 187 75.956 86.866 6.881 1.	2472	CA	HIS	Α						
2477 CG HIS A 183 64.099 91.086 6.806 1.00 29.04 2478 NDI HIS A 183 63.217 90.679 5.835 1.00 29.33 2482 NEZ HIS A 183 61.982 90.944 6.226 1.00 30.87 2486 NEZ HIS A 183 62.033 91.486 7.429 1.00 30.69 2486 C HIS A 183 67.598 89.588 7.410 1.00 29.52 2487 O HIS A 183 68.261 90.375 6.732 1.00 29.82 2498 N VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184	2474	CB	HIS	А	183			6.688	1.00	29.50
2478 ND1 HIS A 183 63.217 90.679 5.835 1.00 29.33 2480 CE1 HIS A 183 61.982 90.944 6.226 1.00 30.87 2482 NE2 HIS A 183 62.033 91.486 7.429 1.00 30.69 2486 CD2 HIS A 183 63.346 91.580 7.816 1.00 30.69 2486 C HIS A 183 668.261 90.375 6.732 1.00 29.56 2487 O HIS A 183 668.261 90.375 6.732 1.00 29.52 2490 CA VAL A 184 68.136 88.569 8.067 1.00 29.52 2490 CA VAL A 184 69.976 87.488 9.352 1.00 29.29 2494 CG1 VAL A 184 69.976 87.488 9.352 1.00 29.29 2494 CG1 VAL A 184 69.976 87.488 9.352 1.00 29.29 2495 CG2 VAL A 184 69.976 87.488 9.352 1.00 29.29 2496 CG2 VAL A 184 69.976 87.904 10.659 1.00 29.32 2498 CG2 VAL A 184 69.545 86.033 8.998 1.00 28.66 2502 C VAL A 184 69.586 88.072 6.886 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.74 2507 CB PRO A 185 71.501 88.441 6.037 1.00 29.74 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.3565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.217 88.146 5.458 1.00 29.72 2510 CG PRO A 185 73.369 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.317 85.896 6.224 1.00 29.23 2516 C PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 72.448 86.659 5.266 1.00 29.23 2518 N LEU A 186 73.319 89.766 6.277 1.00 30.90 2516 C PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 73.317 85.896 6.224 1.00 30.90 2520 CA LEU A 186 73.604 83.417 1.548 1.00 30.90 2521 CG LEU A 186 73.604 83.417 1.548 1.00 30.90 2522 CB LEU A 186 73.695 84.765 2.281 1.00 30.90 2523 CG LEU A 186 73.695 84.765 2.281 1.00 30.74 2533 CB LEU A 186 73.875 84.071 4.670 1.00 30.74 2533 N ASP A 187 75.951 83.903 5.945 1.00 31.77 2545 OD1 ASP A 187 75.953 84.667 6.143 1.00 32.58 2549 N ASP A 187 75.953 86.666 6.881 1.00 37.70 2546 OD2 ASP A 187 75.953 86.666 6.881 1.00 37.70 2546 OD2 ASP A 187 75.963 86.666 6.881 1.00 37.70 2547 C ALA A 188 73.271 85.624 9.641 1.00 31.36 2549 N ALA A 188 73.271 85.624 9.641 1.00 30.46 2557 C ALA A 188 73.271 85.624 9.641 1.00 30.46 2557 C ALA A 188 73.271 85.627 9.082 1.00 30.94	2477	CG	HIS	Α	183	64.099				29.04
2482 NE2 HIS A 183 62.033 91.486 7.429 1.00 30.77 2484 CD2 HIS A 183 63.346 91.580 7.816 1.00 30.57 2486 C HIS A 183 67.598 89.588 7.410 1.00 29.56 2487 O HIS A 183 68.261 90.375 6.732 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.40 2492 CB VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184 69.510 87.904 10.659 1.00 29.72 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 28.66 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.74 2504 N PRO A 18	2478	ND1	HIS	Α	183	63.217	90.679			29.33
2484 CD2 HIS A 183 63.346 91.580 7.816 1.00 30.69 2486 C HIS A 183 67.598 89.588 7.410 1.00 29.56 2487 O HIS A 183 68.261 90.375 6.732 1.00 29.82 2488 N VAL A 184 68.136 88.569 8.067 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.40 2492 CB VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CG1 VAL 1.84 69.645 86.033 8.998 1.00 29.29 22.2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 29.41 25.03 O VAL A 184 69.586 87.448 6.037 1.00 29.72 25.05 A 1.85 72.	2480	CE1	HIS	Α	183	61.982	90.944	6.226	1.00	30.87
2486 C HIS A 183 67.598 89.588 7.410 1.00 29.56 2487 O HIS A 183 68.261 90.375 6.732 1.00 29.82 2488 N VAL A 184 68.136 88.569 8.067 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184 69.976 87.488 9.352 1.00 29.29 2494 CGI VAL A 184 69.516 86.033 8.998 1.00 29.32 2498 CG2 VAL A 184 69.586 87.448 6.037 1.00 29.14 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.70 2504 N PRO A 185 72.217 88.146 5.458 1.00 29.72 2507 CB	2482	NE2	HIS	Α	183	62.033	91.486	7.429	1.00	30.77
2487 O HIS A 183 68.261 90.375 6.732 1.00 29.82 2488 N VAL A 184 68.136 88.569 8.067 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.29 2494 CGI VAL A 184 69.576 87.488 9.352 1.00 29.29 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 29.32 2498 CG2 VAL A 184 69.586 87.448 6.037 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.72 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.72 2505 CA PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CB	2484	CD2	HIS	Α	183	63.346	91.580	7.816	1.00	30.69
2488 N VAL A 184 68.136 88.569 8.067 1.00 29.52 2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.40 2492 CB VAL A 184 69.976 87.488 9.352 1.00 29.29 2494 CGI VAL A 184 69.645 86.033 8.998 1.00 29.32 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.74 2503 O VAL A 185 71.501 88.441 6.037 1.00 29.74 2505 CA PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357	2486	C	HIS	Α	183	67.598	89.588	7.410	1.00	29.56
2490 CA VAL A 184 69.580 88.461 8.215 1.00 29.40 2492 CB VAL A 184 69.976 87.488 9.352 1.00 29.29 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 29.32 2502 C VAL A 184 69.645 86.033 8.998 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.64 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 72.217 88.146 5.458 1.00 29.74 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357	2487	0	HIS	Α	183	68.261	90.375	6.732	1.00	29.82
2492 CB VAL A 184 69.976 87.488 9.352 1.00 29.29 2494 CG1 VAL A 184 69.310 87.904 10.659 1.00 29.32 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.41 2503 O VAL A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 71.501 88.441 6.701 1.00 29.72 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.317	2488	N	VAL	Α	184	68.136	88.569	8.067	1.00	29.52
2494 CG1 VAL A 184 69.310 87.904 10.659 1.00 29.32 2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 28.66 2502 C VAL A 184 70.233 88.072 6.886 1.00 29.41 2504 N PRO A 185 71.501 88.441 6.037 1.00 29.72 2505 CA PRO A 185 72.217 88.146 6.431 1.00 29.74 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357 89.168 7.653 1.00 30.09 2513 CD PRO A 185 72.317 85.896 6.224 1.00 29.95 2517 O PRO A 185 72.317	2490	CA	VAL	Α	184	69.580	88.461	8.215	1.00	29.40
2498 CG2 VAL A 184 69.645 86.033 8.998 1.00 28.66 2502 C VAL A 184 70.233 88.072 6.886 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.64 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.72 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357 89.168 7.653 1.00 30.18 2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.99 2516 C PRO A 185 72.317	2492	CB	VAL	Α	184	69.976	87.488	9.352	1.00	29.29
2502 C VAL A 184 70.233 88.072 6.886 1.00 29.41 2503 O VAL A 184 69.586 87.448 6.037 1.00 29.64 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 72.217 88.146 5.458 1.00 29.72 2507 CB PRO A 185 73.565 88.851 5.643 1.00 30.18 2510 CG PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.317 85.896 6.224 1.00 29.95 2517 O PRO A 186 72.317 85.896 6.224 1.00 30.11 2520 CA LEU A 186 73.010 <	2494					69.310	87.904	10.659	1.00	29.32
2503 O VAL A 184 69.586 87.448 6.037 1.00 29.64 2504 N PRO A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 72.217 88.146 5.458 1.00 29.72 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 72.357 89.168 7.653 1.00 30.08 2516 C PRO A 185 72.317 85.896 6.224 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 30.01 2517 O PRO A 186 73.010 84.873 3.690 1.00 30.11 2520 CB LEU A 186 73.595 <					184	69.645	86.033	8.998	1.00	28.66
2504 N PRO A 185 71.501 88.441 6.701 1.00 29.70 2505 CA PRO A 185 72.217 88.146 5.458 1.00 29.74 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.389 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.09 2517 O PRO A 185 72.448 86.659 5.266 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 73.010 84.873 3.690 1.00 30.11 2520 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2525 CG LEU A 186 73.472 82.695 1.750 1.00 34.56		C	VAL	Α	184	70.233	88.072	6.886	1.00	29.41
2505 CA PRO A 185 72.217 88.146 5.458 1.00 29.74 2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.389 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.317 85.896 6.224 1.00 29.95 2517 O PRO A 186 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 73.3010 84.873 3.690 1.00 30.66 2522 CB LEU A 186 73.595 84.765 2.281 1.00 30.07 2527 CD1 LEU A 186 73.504		0	VAL	Α		69.586		6.037	1.00	29.64
2507 CB PRO A 185 73.565 88.851 5.643 1.00 29.72 2510 CG PRO A 185 73.389 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.448 86.659 5.266 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 73.010 84.873 3.690 1.00 30.11 2520 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2527 CD1 LEU A 186 73.604 83.417 1.548 1.00 31.83 2531 CD2 LEU A 186 73.875			PRO	Α			88.441	6.701	1.00	29.70
2510 CG PRO A 185 73.389 89.766 6.777 1.00 30.18 2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.448 86.659 5.266 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 72.843 86.279 4.059 1.00 30.11 2520 CA LEU A 186 73.010 84.873 3.690 1.00 30.66 2522 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2525 CG LEU A 186 73.604 83.417 1.548 1.00 32.07 2527 CD1 LEU A 186 72.438 82.535 1.942 1.00 31.83 2531 CD2 LEU A 186 73.875 84.071 4.670 1.00 30.74 <										
2513 CD PRO A 185 72.357 89.168 7.653 1.00 30.09 2516 C PRO A 185 72.448 86.659 5.266 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 72.843 86.279 4.059 1.00 30.11 2520 CA LEU A 186 73.010 84.873 3.690 1.00 30.90 2522 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2527 CD1 LEU A 186 73.604 83.417 1.548 1.00 32.07 2527 CD1 LEU A 186 74.931 82.695 1.750 1.00 34.56 2531 CD2 LEU A 186 73.875 84.071 4.670 1.00 30.74 2535 C LEU A 186 73.472 82.997 5.093 1.00 30.94 <										29.72
2516 C PRO A 185 72.448 86.659 5.266 1.00 29.95 2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 72.843 86.279 4.059 1.00 30.11 2520 CA LEU A 186 73.010 84.873 3.690 1.00 30.66 2522 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2525 CG LEU A 186 73.604 83.417 1.548 1.00 32.07 2527 CD1 LEU A 186 74.931 82.695 1.750 1.00 34.56 2531 CD2 LEU A 186 73.875 84.071 4.670 1.00 30.74 2536 O LEU A 186 73.472										30.18
2517 O PRO A 185 72.317 85.896 6.224 1.00 29.23 2518 N LEU A 186 72.843 86.279 4.059 1.00 30.11 2520 CA LEU A 186 73.010 84.873 3.690 1.00 30.66 2522 CB LEU A 186 73.595 84.765 2.281 1.00 30.90 2525 CG LEU A 186 73.604 83.417 1.548 1.00 32.07 2527 CD1 LEU A 186 74.931 82.695 1.750 1.00 34.56 2531 CD2 LEU A 186 73.875 84.071 4.670 1.00 30.74 2536 O LEU A 186 73.472 82.997 5.093 1.00 30.98 2537 N ASP A 187 75.951										
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2557 C ALA A 188 72.627 83.331 8.870 1.00 29.80										
2558 O ALA A 188 72.328 82.505 9.731 1.00 28.47	2557	С	ALA	Α	188	72.627				
	2558	0	ALA	Α	188	72.328	82.505	9.731	1.00	28.47

FIGURE 3 (Cont.) AZ

2559 N	Α	В	C	D	E	F	G	H	I	J
2561 CA LEU A 189 70.902 82.529 7.358 1.00 29.70										
2563 CB LEU A 189 68.870 83.128 5.772 1.00 30.15 2566 CG LEU A 189 68.870 83.128 5.772 1.00 31.79 2572 CD2 LEU A 189 67.958 82.992 4.280 1.00 32.37 2576 C LEU A 189 70.766 80.182 7.923 1.00 27.68 2577 O LEU A 189 70.766 80.182 7.923 1.00 27.68 2578 N GLU A 190 72.539 80.867 6.6712 1.00 28.82 2582 CB GLU A 190 74.362 79.609 5.697 1.00 28.82 2582 CB GLU A 190 74.362 79.609 5.697 1.00 28.82 2582 CB GLU A 190 74.362 79.609 5.697 1.00 29.44 2585 CG GLU A 190 76.119 78.345 4.382 1.00 31.65 2580 CG GLU A 190 76.104 79.127 3.405 1.00 35.05 2590 OE2 GLU A 190 77.126 77.631 4.625 1.00 37.41 2591 C GLU A 190 73.524 78.996 7.972 1.00 28.22 2592 O GLU A 190 73.524 78.996 7.972 1.00 22.22 2592 O GLU A 190 73.524 78.996 7.972 1.00 22.22 2593 N ARG A 191 74.001 79.866 8.856 1.00 27.79 2593 N ARG A 191 74.001 79.866 8.856 1.00 27.79 2595 CA ARG A 191 75.021 80.585 10.988 1.00 23.30 2603 CD ARG A 191 77.323 81.682 11.474 10.0 39.49 2608 CZ ARG A 191 77.323 81.682 11.474 10.0 39.49 2608 CZ ARG A 191 79.520 80.619 11.005 1.00 27.69 2600 CG ARG A 191 79.520 80.619 11.005 1.00 27.69 2600 CG ARG A 191 79.520 80.619 11.005 1.00 26.20 2609 NH ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 27.60 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191 79.520 80.619 11.400 1.00 26.20 2616 O ARG A 191										
2566 CG LEU A										
2568 CD1 LEU A										
2576 CD2 LEU A										
2576 C										
2577										
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2582 CB GLU A 190										
2585 CG GLU A 190										
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FIGURE 3 (Cont.)BA

Α	В	С	D	E	F	G	H	I	J
2669	CZ	ARG	7\	194	76.459	74.147	E 002	1.00	25 12
2670	NH1	ARG		194			5.092		25.12
2673	NH2	ARG			76.120	72.904	5.398	1.00	25.42
				194	76.784	74.455	3.840	1.00	28.83
2676	C	ARG		194	72.780	73.872	10.829	1.00	21.18
2677	0	ARG		194	72.861	72.681	11.071	1.00	20.79
2678	N	HIS	A	195	72.583	74.777	11.784	1.00	21.00
2680	CA	HIS	A	195	72.436	74.337	13.171	1.00	21.63
2682	CB	HIS	A	195	72.773	75.458	14.158	1.00	21.62
2685	CG		A	195	74.232	75.787	14.215	1.00	24.46
2686	ND1	HIS		195	74.944	75.833	15.394	1.00	28.06
2688	CE1	HIS	Α	195	76.201	76.148	15.134	1.00	28.87
2690	NE2	HIS	A	195	76.330	76.304	13.831	1.00	29.50
2692			Α	195	75.113	76.086	13.233	1.00	27.40
2694	С		Α	195	71.050	73.751	13.451	1.00	21.00
2695	0	HIS	Α	195	70.948	72.646	13.985	1.00	20.86
2696	N	LYS	Α	196	69.985	74.462	13.087	1.00	20.63
2698	CA	LYS	Α	196	68.642	74.022	13.489	1.00	20.10
2700	CB	LYS	Α	196	67.590	75.123	13.367	1.00	19.88
2703	CG	LYS	Α	196	66.987	75.363	11.997	1.00	19.59
2706	CD	LYS	A	196	65.944	76.473	12.065	1.00	19.02
2709	CE	LYS	Α	196	65.416	76.847	10.672	1.00	18.63
2712	NZ	LYS	Α	196	64.064	77.494	10.673	1.00	19.09
2716	C	LYS	Α	196	68.215	72.756	12.758	1.00	20.00
2717	0	LYS	Α	196	67.491	71.960	13.307	1.00	20.23
2718	N	THR	Α	197	68.705	72.557	11.539	1.00	19.63
2720	CA	THR	Α	197	68.278	71.433	10.726	1.00	19.13
2722	CB	THR	Α	197	67.408	71.938	9.580	1.00	19.35
2724	OG1	THR	Α	197	66.166	72.400	10.127	1.00	18.33
2726	CG2	THR	Α	197	67.021	70.812	8.618	1.00	18.67
2730	С	THR	Α	197	69.413	70.554	10.226	1.00	19.03
2731	0	THR	Α	197	69.275	69.332	10.223	1.00	18.17
2732	N	GLY	Α	198	70.522	71.167	9.812	1.00	19.30
2734	CA	GLY	Α	198	71.667	70.421	9.316	1.00	19.16
2737	С	GLY		198	72.260	69.466	10.329	1.00	19.28
2738	0	GLY		198	72.580	68.330	9.987	1.00	19.12
2739	N	ALA	Α	199	72.371	69.910	11.576	1.00	19.18
2741	CA	ALA		199	73.129	69.182	12.585	1.00	19.36
2743	CB	ALA		199	73.245	70.005	13.861		19.70
2747	C	ALA		199	72.505	67.816	12.897	1.00	19.34
2748	Ō	ALA		199	73.224	66.830	13.057	1.00	19.28
2749	N	LEU		200	71.177	67.768	12.994	1.00	19.51
2751	CA	LEU		200	70.476	66.522	13.302	1.00	19.63
2753	СВ	LEU		200	69.016	66.775	13.700	1.00	19.77
2756	CG	LEU		200	68.261	65.516	14.183	1.00	20.34
2758		LEU		200	68.918	64.931	15.431		
2762		LEU		200	66.799	65.855	14.449		20.55
2766	C	LEU		200	70.514	65.563	12.125	1.00	19.55
2767	o	LEU		200	70.514	64.336	12.312	1.00	19.72
2768	N	ILE		201	70.462	66.114	10.919	1.00	19.19
2770	CA	ILE		201	70.556	65.299	9.706	1.00	19.51
2772	CB	ILE		201	70.338	66.143	8.471	1.00	19.64
2774	CG1	ILE		201	68.659	66.197	8.372		20.21

FIGURE 3 (Cont.)BB

2777 CD1 ILE A 201 68.149 67.249 7.449 1.00 21.65 2781 CG2 ILE A 201 70.782 65.578 7.169 1.00 20.92 2785 C ILE A 201 71.941 64.661 9.604 1.00 19.17 2786 O ILE A 201 72.066 63.504 9.227 1.00 18.77 2787 N ARG A 202 72.970 65.420 9.963 1.00 19.39 2799 CB ARG A 202 74.323 66.008 10.148 1.00 20.03 2794 CG ARG A 202 75.343 66.008 10.148 1.00 20.03 2794 CG ARG A 202 77.777 66.638 10.165 1.00 20.03 2794 CG ARG A 202 77.777 66.638 10.165 1.00 20.03 2794 CG ARG A 202 77.777 66.638 10.165 1.00 20.03 2802 CZ ARG A 202 77.824 67.265 11.473 1.00 23.53 2802 CZ ARG A 202 77.824 67.265 11.473 1.00 23.53 2802 CZ ARG A 202 79.445 68.805 13.012 1.00 23.66 2806 NH1 ARG A 202 79.445 68.805 13.012 1.00 23.66 2806 NH2 ARG A 202 74.453 63.843 11.113 1.00 19.73 2810 C ARG A 202 75.153 62.859 10.891 1.00 25.66 2813 CA ALA A 203 73.741 64.027 12.226 1.00 19.24 2813 CA ALA A 203 73.741 64.027 12.226 1.00 19.64 2813 CA ALA A 203 73.741 64.027 12.226 1.00 19.64 2820 C ALA A 203 73.741 64.027 12.226 1.00 18.65 2815 CB ALA A 203 73.736 60.644 13.210 1.00 18.60 2820 C ALA A 203 73.582 60.644 13.210 1.00 18.03 2821 N ALA A 203 73.582 60.644 13.210 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 18.04 2825 CB ALA A 204 70.266 60.486 10.588 1.00 10.01 18.04 2825 CB ALA A 204 70.266 60.868	Α	В	С	D	E		F	G		Н		I	J
2781 CG2 ILE A 201 70.782 65.578 7.169 1.00 20.99 2786 C ILE A 201 71.941 64.661 9.604 1.00 19.17 2787 N ARG A 202 72.970 65.420 9.963 1.00 19.39 2789 CA ARG A 202 75.343 66.008 10.148 1.00 20.03 2797 CD ARG A 202 76.774 65.526 10.119 1.00 21.06 2797 CD ARG A 202 77.777 66.538 10.165 1.00 20.98 2800 NE ARG A 202 78.641 68.254 11.789 1.00 23.66 2805 NH1 ARG A 202 78.455 68.815 10.891 1.00 26.69 2806 NH2 ARG A 202 75.153 62.859 10.91 10.00 26.69 2806 NH2 </td <td></td> <td>an •</td> <td></td> <td>_</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>_</td> <td></td> <td></td> <td></td>		an •		_						_			
2785 C ILE A 201 71.941 64.661 9.604 1.00 19.17 2786 O LLE A 201 72.066 63.504 9.227 1.00 18.77 2787 N ARG A 202 74.323 64.891 10.001 1.00 19.72 2791 CB ARG A 202 76.744 65.526 10.119 1.00 21.03 2797 CD ARG A 202 77.777 66.638 10.165 1.00 23.53 2800 NE ARG A 202 78.617 68.294 11.789 1.00 23.53 2803 NH1 ARG A 202 78.617 68.294 11.73 1.00 23.53 2806 NH2 ARG A 202 79.445 68.800 13.012 1.00 26.69 2806 NH2 ARG A 202 75.153 62.859 10.935 1.00 19.84 2811 N													
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2841 CG2 VAL A 205 73.476 61.057 6.930 1.00 17.58 2845 C VAL A 205 75.314 59.238 9.852 1.00 18.69 2846 O VAL A 205 75.716 58.086 9.677 1.00 20.23 2847 N ARG A 206 75.783 60.032 10.808 1.00 18.74 2849 CA ARG A 206 76.862 59.629 11.702 1.00 18.76 2851 CB ARG A 206 77.274 60.778 12.615 1.00 18.76 2854 CG ARG A 206 78.157 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.71 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2861 NH1	2835	CB	VAL	Α	205	74	.659	60.	714	7.	874	1.00	18.22
2845 C VAL A 205 75.314 59.238 9.852 1.00 18.69 2846 O VAL A 205 75.716 58.086 9.677 1.00 20.23 2847 N ARG A 206 75.783 60.032 10.808 1.00 18.74 2849 CA ARG A 206 76.862 59.629 11.702 1.00 18.76 2851 CB ARG A 206 77.274 60.778 12.615 1.00 18.76 2854 CG ARG A 206 78.457 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.71 2857 CD ARG A 206 79.481 63.857 12.167 1.00 21.03 2860 NE ARG A 206 80.008 64.936 12.737 1.00 22.08 2863 NH1	2837	CG1	VAL	Α	205	75	.791	60.	079	7.	109	1.00	18.92
2846 O VAL A 205	2841	CG2	VAL	Α	205	73	.476	61.	057	6.	930	1.00	17.58
2847 N ARG A 206 75.783 60.032 10.808 1.00 18.74 2849 CA ARG A 206 76.862 59.629 11.702 1.00 18.96 2851 CB ARG A 206 77.274 60.778 12.615 1.00 18.76 2854 CG ARG A 206 78.157 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.66 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90	2845	С	VAL	Α	205	75	.314	59.2	238	9.	852	1.00	18.69
2849 CA ARG A 206 76.862 59.629 11.702 1.00 18.96 2851 CB ARG A 206 77.274 60.778 12.615 1.00 18.76 2854 CG ARG A 206 78.157 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.66 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90	2846	0	VAL	Α	205	75	.716	58.	086	9.	677	1.00	20.23
2851 CB ARG A 206 77.274 60.778 12.615 1.00 18.76 2854 CG ARG A 206 78.157 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.66 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 80.903 65.660 12.079 1.00 21.63 2870 O ARG A 206 76.481 58.427 12.549 1.00 19.18 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90								60.0	032	10.	808	1.00	18.74
2854 CG ARG A 206 78.157 61.792 11.948 1.00 19.71 2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.66 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 74.790 <td></td> <td></td> <td></td> <td></td> <td></td> <td>76</td> <td>.862</td> <td></td> <td></td> <td></td> <td></td> <td>1.00</td> <td></td>						76	.862					1.00	
2857 CD ARG A 206 78.477 63.008 12.803 1.00 19.66 2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90										12.	615	1.00	18.76
2860 NE ARG A 206 79.481 63.857 12.167 1.00 21.03 2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2862 CZ ARG A 206 80.008 64.936 12.737 1.00 22.60 2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 74.453 <td></td>													
2863 NH1 ARG A 206 79.659 65.289 13.965 1.00 22.08 2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU </td <td></td>													
2866 NH2 ARG A 206 80.903 65.660 12.079 1.00 21.63 2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2869 C ARG A 206 76.481 58.427 12.549 1.00 19.18 2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2870 O ARG A 206 77.283 57.530 12.757 1.00 18.61 2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 <td></td>													
2871 N LEU A 207 75.244 58.394 13.014 1.00 19.73 2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2873 CA LEU A 207 74.790 57.288 13.850 1.00 20.29 2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2875 CB LEU A 207 73.426 57.600 14.481 1.00 20.21 2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2878 CG LEU A 207 73.432 58.067 15.944 1.00 21.69 2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2880 CD1 LEU A 207 74.453 59.147 16.210 1.00 22.70 2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2884 CD2 LEU A 207 72.044 58.554 16.298 1.00 23.52 2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2888 C LEU A 207 74.715 56.013 13.013 1.00 20.31 2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													
2889 O LEU A 207 75.049 54.941 13.486 1.00 19.90													

FIGURE 3 (Cont.)BC

Α	В	С	D	E	F	G	H	I	J
			_						
2892	CA	GLY		208	74.297	55.000	10.861		21.15
2895	C	GLY		208	75.703	54.457	10.656		21.20
2896	0	GLY		208	75.933	53.240	10.737	1.00	22.15
2897	N	ALA		209	76.643	55.362	10.419	1.00	21.27
2899	CA	ALA		209	78.046	55.006	10.215	1.00	22.05
2901	CB	ALA		209	78.813	56.193	9.733	1.00	21.96
2905	C	ALA		209	78.700	54.419	11.480	1.00	22.41
2906	0	ALA		209	79.383	53.398	11.411	1.00	22.53
2907	N	LEU		210	78.471	55.041	12.635	1.00	22.29
2909	CA	LEU		210	79.090	54.580	13.877		22.51
2911	CB	LEU		210	78.775	55.522	15.039		22.37
2914	CG	LEU		210	79.513	56.853	14.977		22.40
2916	CD1	LEU		210	78.845	57.900 56.689	15.863	1.00	22.42
2920 2924	CD2 C	LEU		210	81.004		15.372		22.32
2924		LEU		210	78.642	53.168	14.213	1.00	23.22
2925 2926	O N	SER		210 211	79.383	52.408 52.809	14.830	1.00	23.30
2928	N CA	SER		211	77.430 76.914	51.469	13.786		
2920	CB	SER		211	75.478	51.469	13.999 13.496	1.00	
2933	OG	SER		211	75.478	51.347	12.104	1.00	24.10 25.59
2935	C	SER		211	77.764	50.397	13.335		24.24
2936	0	SER		211	77.744	49.254	13.333		23.60
2937	N	ALA		212	78.464	50.782	12.269		24.79
2939	CA	ALA		212	79.332	49.906	11.496	1.00	
2941	CB	ALA		212	79.361	50.376	10.050	1.00	
2945	C	ALA		212	80.762	49.837	12.044	1.00	26.25
2946	0	ALA		212	81.602	49.130	11.490	1.00	27.04
2947	N	GLY		212	81.051	50.586	13.100	1.00	
2949	CA	GLY		213	82.373	50.574	13.692	1.00	
2952	C	GLY		213	83.427	51.209	12.809	1.00	
2953	ō	GLY		213	83.193	52.242	12.199	1.00	27.58
2954	N	ASP		214	84.584	50.570	12.718		28.92
2956	CA	ASP		214	85.758	51.188	12.105		29.67
2958	CB	ASP		214	86.993	50.294	12.281	1.00	30.31
2961	CG	ASP		214	87.596	50.413	13.666	1.00	33.03
2962		ASP		214	88.445	49.568	14.020	1.00	37.45
2963		ASP		214	87.285	51.318	14.478	1.00	35.85
2964	C	ASP		214	85.530	51.523	10.650		29.40
2965	0	ASP		214	85.907	52.596	10.203		29.23
2966	N	LYS		215	84.879	50.625	9.921		29.50
2968	CA	LYS		215	84.593	50.862	8.505		29.92
2970	CB	LYS		215	84.019	49.610	7.839		30.45
2973	CG	LYS		215	85.103	48.766	7.182		33.43
2976	CD	LYS		215	84.685	47.310	6.964		36.17
2979	CE	LYS		215	85.888	46.439	6.568		37.55
2982	NZ	LYS		215	85.967	45.213	7.416		39.13
2986	С	LYS		215	83.672	52.076	8.312		29.02
2987	0	LYS		215	83.851	52.860	7.384		27.84
2988	N	GLY		216	82.696	52.241	9.198		28.66
2990	CA	GLY		216	81.855	53.429	9.162		28.17
2993	C	GLY	A	216	82.647	54.692	9.471	1.00	27.77
2994	0	GLY	Α	216	82.503	55.719	8.812	1.00	27.08

FIGURE 3 (Cont.)BD

Α	В	С	D	E		F		G	I	Ŧ	I	J
2995	N	ARG	Δ	217	s	33.498	,	54.609	7 (0.482	1.0	27.98
2997	CA	ARG		217		34.306		55.751		0.900	1.0	
2999	CB	ARG		217		35.165		55.391		2.106	1.0	
3002	CG	ARG		217		34.449		55.520		3.428	1.0	
3005	CD	ARG		217		35.328		55.173		1.580	1.0	
3008	NE	ARG		217		34.577		55.110		5.826	1.0	
3010	CZ	ARG		217		34.375		56.148		5.637	1.0	
3011	NH1	ARG		217		34.836						
3011	NH2	ARG		217		33.671		57.359 55.980		5.334	1.0	
3017	C	ARG		217				56.266		7.743	1.0	
3017	0	ARG		217		35.201				9.783	1.0	
3019	N	ARG		217		35.367		57.476		9.645	1.0	
	CA					35.752		55.354		3.978	1.0	
3021 3023	CB	ARG ARG		218 218		36.622		55.726		7.853	1.0	
	CG	ARG				37.268		54.483		7.223	1.0	
3026				218		38.351		53.812		3.069	1.0	
3029	CD	ARG		218		38.273		52.280		3.115	1.0	
3032	NE	ARG		218		38.914		51.617		5.975	1.0	
3034	CZ NH1	ARG ARG		218		88.318		51.290		5.817	1.0	
3035	NH2			218		39.023		50.681		1.862	1.0	
3038		ARG		218		37.037		51.564		5.587	1.0	
3041 3042	C 0	ARG		218 218		35.866		56.481		5.765	1.0	
3042	N	ARG				36.460		57.283		5.034	1.0	
3045	CA	ALA ALA		219 219		34.565		56.209		6.646	1.0	
3045	CB	ALA		219		33.720		56.894		5.669	1.0	
3047	C	ALA				32.532		56.030		5.313	1.0	
3051	0	ALA		219 219		33.234		58.253		5.142	1.0	
3052	N	LEU		220		32.710 33.394		59.018 58.543		5.344	1.0	
3055	CA	LEU		220		32.807		59.736		7.433 3.036	$\frac{1.0}{1.0}$	
3057	СВ	LEU		220		33.061		59.804		9.546	1.0	
3060	CG	LEU		220		32.127		58.960		0.416	1.0	
3062	CD1	LEU		220		32.573		59.004		L.889	1.0	
3066	CD2	LEU		220		30.677		59.411		0.271	1.0	
3070	C	LEU		220		33.226		51.045		7.400	1.0	
3071	ō	LEU		220		32.380		51.901		7.232	1.0	
3072	N	PRO		221		34.502		51.248		7.067	1.0	
3073	CA	PRO		221		34.879		52.502		5.399	1.0	
3075	СВ	PRO		221		36.349		52.269		5.006		26.54
3078	CG	PRO		221		36.853		51.366		7.081		27.08
3081	CD	PRO		221		35.685		50.415		7.352	1.0	
3084	C	PRO		221		33.996		52.758		5.195	1.0	
3085	ō	PRO		221		33.479		53.859		5.044		26.22
3086	N	VAL		222		33.770		51.735		1.381		24.71
3088	ÇA	VAL		222		32.965		51.910		3.181		24.34
3090	CB	VAL		222		33.272		50.835		2.139		24.09
3092	CG1	VAL		222		32.302		50.927		0.999	1.0	
3096	CG2	VAL		222		34.718		50.988		1.655		25.44
3100	C	VAL		222		31.465		51.955		3.470		23.78
3101	0	VAL		222		30.754		52.771		2.885	1.0	
3102	N	LEU		223		30.978		51.096		1.362	1.0	
3104	CA	LEU		223		79.552		51.118		1.707		22.90
3106	CB	LEU	Α	223		79.179		9.955		5.627		23.13

FIGURE 3 (Cont.)BE

A	В	С	D	E	F	G	H	I	J
3109	CG	LEU	Δ	223	79.130	58.583	4.947	1 00	22.78
3111	CD1	LEU		223	79.022	57.462	5.987		23.57
3115	CD2	LEU		223	77.991	58.484	3.975		23.72
3119	C	LEU		223	79.159	62.441	5.346	1.00	
	0	LEU		223	78.023				
3120						62.903	5.182	1.00	22.74
3121	N	ASP		224	80.081	63.036	6.093	1.00	23.24
3123	CA	ASP		224	79.838	64.328	6.722	1.00	23.61
3125	CB	ASP		224	81.028	64.753	7.588	1.00	
3128	CG	ASP		224	81.009	64.118	8.974	1.00	
3129	OD1	ASP		224	79.961	63.561	9.379	1.00	
3130	OD2	ASP		224	81.989	64.158	9.749	1.00	27.02
3131	C	ASP		224	79.568	65.385	5.654	1.00	
3132	0	ASP		224	78.630	66.175	5.772		22.89
3133	N	LYS		225	80.373	65.377	4.599		23.58
3135	CA	LYS		225	80.234	66.391	3.557		24.32
3137	CB	LYS		225	81.439	66.381	2.594	1.00	24.94
3140	CG	LYS		225	82.825	66.478	3.298	1.00	27.64
3143	CD	LYS	Α	225	83.113	67.828	4.009	1.00	31.84
3146	CE	LYS	Α	225	83.516	67.719	5.546	1.00	32.28
3149	NZ	LYS	Α	225	84.063	66.374	6.064	1.00	30.63
3153	C	LYS	Α	225	78.901	66.207	2.842	1.00	23.43
3154	0	LYS	Α	225	78.205	67.177	2.548	1.00	23.79
3155	N	TYR	Α	226	78.521	64.955	2.612	1.00	22.64
3157	CA	TYR	Α	226	77.214	64.632	2.063	1.00	21.59
3159	CB	TYR	Α	226	77.075	63.114	1.881	1.00	21.93
3162	CG	TYR	Α	226	75.645	62.633	1.753	1.00	20.62
3163	CD1	TYR	Α	226	75.021	62.606	0.523	1.00	21.37
3165	CE1	TYR	Α	226	73.736	62.160	0.386	1.00	20.90
3167	CZ	TYR	Α	226	73.030	61.727	1.487	1.00	20.66
3168	OH	TYR	Α	226	71.737	61.289	1.311	1.00	21.67
3170	CE2	TYR	Α	226	73.617	61.727	2.730	1.00	21.12
3172	CD2	TYR	Α	226	74.933	62.174	2.862	1.00	20.69
3174	С	TYR	Α	226	76.098	65.121	2.979	1.00	21.19
3175	0	TYR	Α	226	75.156	65.754	2.523	1.00	21.30
3176	N	ALA	Α	227	76.208	64.804	4.261	1.00	20.68
3178	CA	ALA	Α	227	75.173	65.126	5.240	1.00	20.41
3180	CB	ALA	Α	227	75.503	64.513	6.581	1.00	
3184	С	ALA		227	75.007	66.627	5.390		20.36
3185	0	ALA		227	73.893	67.123	5.485		19.95
3186	N	GLU		228	76.132	67.326	5.407		20.85
3188	CA	GLU		228	76.160	68.786	5.503		21.65
3190	СВ	GLU		228	77.601	69.285	5.581		21.59
3193	CG	GLU		228	78.225	69.020	6.940		23.51
3196	CD	GLU		228	79.737	68.868	6.911		25.72
3197		GLU		228	80.292	68.333	7.899		25.16
3198	OE2	GLU		228	80.367	69.272	5.910		28.53
3199	C	GLU		228	75.411	69.428	4.340		21.53
3200	ō	GLU		228	74.644	70.370	4.532		22.09
3201	N	SER		229	75.600	68.899	3.141		21.49
3203	CA	SER		229	74.922	69.459	1.985	1.00	
3205	СВ	SER		229	75.598	69.036	0.695		21.17
3208	OG	SER		229	76.870	69.647	0.589		22.38
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FIGURE 3 (Cont.) BF

A	В	С	D	E	F	G	Н	I	J
3210	С	SER	Α	229	73.432	69.119	1.967	1.00	21.32
3211	Ō	SER		229	72.629	69.993	1.719	1.00	20.51
3212	N		A	230	73.044	67.871	2.238	1.00	21.52
3214	CA	ILE	Α	230	71.610	67.562	2.236	1.00	21.70
3216	CB		Α	230	71.318	66.049	2.154	1.00	21.58
3218	CG1	ILE	Α	230	71.881	65.279	3.347		22.85
3221	CD1		Α	230	71.069	64.038	3.669	1.00	22.81
3225	CG2	ILE	Α	230	71.815	65.486	0.849	1.00	21.97
3229	С	ILE	Α	230	70.874	68.190	3.421		21.12
3230	0	ILE	Α	230	69.684	68.467	3.337	1.00	21.31
3231	N	GLY	Α	231	71.583	68.412	4.520	1.00	21.08
3233	CA	GLY	A	231	70.983	68.977	5.714	1.00	21.32
3236	С	GLY	Α	231	70.607	70.441	5.534	1.00	21.14
3237	0	GLY	Α	231	69.514	70.877	5.917	1.00	21.86
3238	N	LEU	Α	232	71.513	71.205	4.939	1.00	21.35
3240	CA	LEU	Α	232	71.214	72.583	4.595	1.00	21.18
3242	CB	LEU	Α	232	72.467	73.318	4.127	1.00	21.49
3245	CG	LEU	Α	232	72.250	74.769	3.712	1.00	21.63
3247	CD1	LEU	Α	232	71.601	75.564	4.829	1.00	22.56
3251	CD2	LEU	A	232	73.571	75.361	3.320	1.00	23.37
3255	С	LEU	Α	232	70.134	72.604	3.521	1.00	20.95
3256	0	LEU	A	232	69.171	73.324	3.659	1.00	20.57
3257	N	ALA	Α	233	70.270	71.766	2.488	1.00	20.80
3259	CA	ALA	Α	233	69.271	71.677	1.424	1.00	20.94
3261	CB	ALA	Α	233	69.674	70.639	0.373	1.00	21.23
3265	С	ALA	Α	233	67.885	71.350	1.966	1.00	20.81
3266	0	ALA	A	233	66.878	71.812	1.442	1.00	20.67
3267	N	PHE	A	234	67.840	70.554	3.029	1.00	20.67
3269	CA	PHE	Α	234	66.568	70.166	3.634	1.00	20.70
3271	CB	PHE	Α	234	66.798	69.201	4.785	1.00	20.78
3274	CG	PHE	Α	234	65.600	68.375	5.131	1.00	22.14
3275	CD1	PHE	A	234	65.546	67.041	4.768	1.00	23.74
3277	CE1	PHE	Α	234	64.455	66.267	5.103	1.00	25.17
3279	CZ		A	234	63.407	66.817	5.797	1.00	23.85
3281	CE2	PHE	Α	234	63.462	68.143	6.173	1.00	23.26
3283	CD2	PHE	A	234	64.551	68.907	5.851	1.00	21.11
3285	C		A	234	65.812	71.378	4.147		20.30
3286	0	PHE		234	64.590	71.496	3.939		19.63
3287	N	GLN		235	66.523	72.269	4.835		20.63
3289	CA	GLN		235	65.874	73.456	5.381		21.12
3291	CB	GLN		235	66.699	74.091	6.503		21.39
3294	CG	GLN		235	65.944	75.205	7.276		21.45
3297	CD	GLN		235	64.668	74.715	7.926		23.00
3298		GLN		235	64.650	73.654	8.548		23.23
3299		GLN		235	63.595	75.490	7.795		20.99
3302	C	GLN		235	65.546	74.494	4.300		21.77
3303	O N	GLN		235	64.511	75.148	4.375		22.39
3304	N Ca	VAL		236	66.402	74.641	3.299		22.51
3306	CA	VAL		236	66.066	75.543	2.184		22.92
3308	CB CG1	VAL VAL		236	67.260	75.840	1.212		23.27
3310 3314		VAL		236	68.054 66.794	74.664	0.922		26.25
3314	CGZ	٧AL	M	236	66.794	76.486	-0.102	1.00	23.71

FIGURE 3 (Cont.)BG

A	В	С	D	E	F	G	Н	I	J
3318	С	VAL	Α	236	64.79	94 75.075	1.478	1.00	22.84
3319	0	VAL		236	63.93			1.00	
3320	N	GLN		237	64.63			1.00	
3322	CA	GLN		237	63.41			1.00	
3324	CB	GLN		237	63.53			1.00	
3327	CG	GLN		237	62.27			1.00	
3330	CD	GLN		237	62.05			1.00	
3331	0E1	GLN		237	62.81			1.00	
3332	NE2	GLN		237	61.02			1.00	
3335	C	GLN		237	62.24			1.00	
3336	0	GLN		237	61.14			1.00	
3337	N	ASP		238	62.46			1.00	
3339	CA	ASP		238	61.40				
3341	CB	ASP		238	61.89			1.00	
3344	CG	ASP		238	60.80			1.00	
3345	OD1			238	59.87				
3346	OD2	ASP		238	60.77			1.00	
3347	C	ASP		238				1.00	
3347	0	ASP		238	60.90 59.70			1.00	
3349	N	ASP	A	239				1.00	
3351	CA	ASP	A	239	61.82			1.00	
3353	CB	ASP		239	61.44			1.00	
3356	CG	ASP		239	62.67 63.43			1.00	
3357	OD1			239				1.00	
3357	OD1	ASP		239	62.96			1.00	
3359	C C	ASP			64.54			1.00	
				239	60.67			1.00	
3360	O N	ASP		239	59.71			1.00	
3361	N	ILE		240	61.12			1.00	
3363	CA	ILE		240	60.50			1.00	
3365	CB	ILE		240	61.35			1.00	
3367	CG1	ILE		240	62.59				25.00
3370	CD1 CG2	ILE		240	63.69			1.00	
3374 3378	C	ILE ILE		240 240	60.54			1.00	
3379	0	ILE			59.09			1.00	
3380	N	LEU		240 241	58.16			1.00	
3382	CA	LEU		241	58.92 57.60			1.00	
3384	CB	LEU		241	57.60			1.00	25.47 25.41
3387	CG	LEU		241	58.36				26.20
3389	CD1			241	58.59				26.20
3393		LEU		241	57.52				26.19
3397	C	LEU		241	56.67				25.82
3398	o	LEU		241	55.46				26.02
3399	N	ASP		242	57.23				26.02
3401	CA	ASP		242	56.42				27.02
3403	CB	ASP		242	57.23				26.69
3406	CG	ASP		242	56.39				28.82
3407		ASP		242	55.88				29.75
3408		ASP		242	56.14				31.49
3409	C	ASP		242	55.76				27.65
3410	o	ASP		242	54.62				28.08
3411	N	VAL		243	56.48				28.57
			-						

FIGURE 3 (Cont.)BH

A	В	С	D	E	F	G	H	I	J
2412	C 3	7.7.7.T	_	242	FF 040				
3413	CA	VAL		243	55.949	79.838	0.542	1.00	
3415	CB	VAL		243	57.091	80.577	-0.188		29.49
3417	CG1	VAL		243	56.537	81.656	-1.140	1.00	29.98
3421	CG2	VAL		243	58.062	81.200	0.825	1.00	29.51
3425	С	VAL		243	54.951	79.248	-0.477	1.00	30.63
3426	0	VAL		243	53.791	79.669	-0.525	1.00	30.78
3427	N	VAL		244	55.388	78.253	-1.250	1.00	•
3429	CA	VAL		244	54.642	77.785	-2.427		32.17
3431	CB	VAL		244	55.605	77.525	-3.617		32.40
3433	CG1	LAV		244	56.588	78.680	-3.768		32.66
3437	CG2	VAL		244	56.349	76.185	-3.462		32.82
3441	С	VAL		244	53.766	76.543	-2.233		32.47
3442	0	VAL		244	52.963	76.204	-3.110	1.00	32.70
3443	N	GLY		245	53.915	75.854	-1.105		32.77
3445	CA	GLY		245	53.200	74.611	-0.879	1.00	33.14
3448	С	GLY	Α	245	51.784	74.871	-0.407	1.00	33.82
3449	0	GLY		245	51.515	75.920	0.162	1.00	34.10
3450	N	ASP	Α	246	50.887	73.920	-0.656	1.00	34.38
3452	CA	ASP	Α	246	49.489	73.995	-0.211	1.00	34.75
3454	CB	ASP		246	48.602	73.159	-1.151	1.00	35.30
3457	CG	ASP		246	47.185	73.699	-1.272	1.00	38.65
3458	OD1	ASP		246	46.738	73.925	-2.425	1.00	42.04
3459		ASP	Α	246	46.433	73.914	-0.284	1.00	42.91
3460	С	ASP	Α	246	49.431	73.410	1.198	1.00	33.97
3461	0	ASP	Α	246	50.088	72.411	1.456	1.00	33.79
3462	N	THR	A	247	48.643	74.009	2.089	1.00	33.08
3464	CA	THR	Α	247	48.489	73.517	3.465	1.00	32.87
3466	CB	THR	Α	247	47.476	74.394	4.249	1.00	32.46
3468	OG1	THR	Α	247	48.002	75.710	4.420	1.00	32.70
3470	CG2	THR	Α	247	47.288	73.901	5.684	1.00	32.42
3474	C	THR	A	247	48.061	72.041	3.542	1.00	32.67
3475	0	THR	Α	247	48.561	71.297	4.377	1.00	32.65
3476	N	ALA		248	47.141	71.617	2.677	1.00	32.34
3478	CA	ALA	Α	248	46.651	70.240	2.709	1.00	32.14
3480	CB	ALA	Α	248	45.388	70.095	1.857	1.00	32.51
3484	С	ALA		248	47.724	69.228	2.271	1.00	31.60
3485	0	ALA	Α	248	47.692	68.073	2.678	1.00	31.38
3486	N	THR		249	48.668	69.666	1.447	1.00	31.12
3488	CA	THR		249	49.785	68.815	1.025		31.09
3490	CB	THR		249	50.269	69.251	-0.371		31.32
3492	OG1	THR		249	49.192	69.112	-1.313		33.79
3494	CG2	THR		249	51.348	68.308	-0.917	1.00	31.41
3498	С	THR		249	50.943	68.825	2.045		30.23
3499	0	THR		249	51.483	67.768	2.391		30.03
3500	N	LEU		250	51.312	70.017	2.520	1.00	29.30
3502	CA	LEU		250	52.358	70.175	3.539		28.64
3504	CB	LEU		250	52.668	71.653	3.766	1.00	
3507	CG	LEU		250	53.253	72.412	2.577	1.00	
3509		LEU		250	53.329	73.903	2.883		29.07
3513		LEU		250	54.620	71.880	2.197		29.56
3517	C	LEU		250	52.007	69.554	4.880		27.73
3518	0	LEU	Α	250	52.877	69.038	5.578	1.00	27.92

FIGURE 3 (Cont.)BI

Α	В	С	D	E	F	, G	Н	I	J
3519	N	GLY	Α	251	50.732	69.613	5.240	1.00	26.76
3521	CA	GLY		251	50.277	69.195	6.546		26.19
3524	C	GLY		251	50.485	70.266	7.601	1.00	25.80
3525	ō	GLY		251	50.150	70.053	8.757	1.00	24.95
3526	N	LYS		252	51.071	71.388	7.197	1.00	25.86
3528	CA	LYS		252	51.273	72.556	8.052	1.00	26.53
3530	СВ	LYS		252	52.701	72.588	8.628	1.00	25.80
3533	CG	LYS		252	53.804	72.498	7.579	1.00	
3536	CD	LYS		252	55.183	72.231	8.200	1.00	23.61
3539	CE	LYS	Α	252	56.297	72.507	7.205	1.00	22.86
3542	NZ	LYS		252	57.604	71.866	7.602	1.00	21.94
3546	С	LYS		252	50.992	73.813	7.223	1.00	27.55
3547	0	LYS		252	51.046	73.781	5.982	1.00	28.12
3548	N	ARG		253	50.721	74.918	7.905	1.00	28.61
3550	CA	ARG		253	50.217	76.128	7.249	1.00	29.63
3552	СВ	ARG		253	49.658	77.096	8.287	1.00	30.10
3555	CG	ARG		253	48.370	76.612	8.875	1.00	32.12
3558	CD	ARG		253	47.441	77.693	9.362	1.00	35.28
3561	NE	ARG		253	46.380	77.104	10.175	1.00	38.07
3563	CZ	ARG		253	45.308	76.476	9.688	1.00	40.08
3564	NH1	ARG		253	45.095	76.378	8.376	1.00	39.60
3567	NH2	ARG		253	44.419	75.962	10.533	1.00	40.97
3570	С	ARG		253	51.223	76.852	6.360	1.00	29.71
3571	ō	ARG		253	52.306	77.274	6.806	1.00	29.38
3572	N	GLN		254	50.847	76.966	5.084	1.00	30.10
3574	CA	GLN		254	51.544	77.794	4.108	1.00	29.94
3576	CB	GLN		254	50.816	77.731	2.754	1.00	30.17
3579	CG	GLN		254	51.436	78.643	1.649	1.00	31.83
3582	CD	GLN		254	50.618	78.716	0.357	1.00	34.25
3583	QE1	GLN	Α	254	51.157	79.057	-0.705	1.00	35.57
3584	NE2	GLN		254	49.333	78.396	0.439	1.00	35.68
3587	С	GLN		254	51.586	79.238	4.601	1.00	29.79
3588	0	GLN	Α	254	50.625	79.733	5.193	1.00	29.82
3589	N	GLY	A	255	52.705	79.907	4.369	1.00	29.23
3591	CA	GLY		255	52.843	81.298	4.740	1.00	29.36
3594	С	GLY	Α	255	53.063	81.513	6.230	1.00	29.17
3595	0	GLY		255	52.963	82.630	6.708	1.00	28.41
3596	N	ALA	Α	256	53.372	80.453	6.971		29.32
3598	CA	ALA		256	53.670	80.594	8.395		29.31
3600	CB	ALA		256	53.865	79.216	9.032		29.54
3604	С	ALA	Α	256	54.900	81.481	8.638		29.48
3605	0	ALA	A	256	54.915	82.276	9.569	1.00	30.09
3606	N	ASP	Α	257	55.925	81.350	7.805		29.41
3608	CA	ASP	Α	257	57.170	82.079	8.006	1.00	29.43
3610	CB	ASP	Α	257	58.242	81.581	7.053	1.00	29.35
3613	CG	ASP	Α	257	58.770	80.208	7.420	1.00	28.93
3614	OD1	ASP		257	58.493	79.724	8.552		27.10
3615	OD2	ASP	A	257	59.480	79.562	6.613		25.07
3616	C	ASP	A	257	56.992	83.576	7.772		30.15
3617	0	ASP	A	257	57.516	84.404	8.505		28.74
3618	N	GLN	Α	258	56.258	83.887	6.717		31.27
3620	CA	GLN	A	258	56.003	85.254	6.311	1.00	32.11

FIGURE 3 (Cont.)BJ

Α	В	C	D	E	F	G	Н	I	J
3622	CB I	BGLN	A	258	55.223	85.271	4.997	0.35	32.00
3623		AGLN		258	55.313	85.259	4.930		32.18
3628		BGLN		258	55.115	86.632	4.342	0.35	31.76
3629		AGLN		258	56.317	84.920	3.801	0.65	32.43
3634		BGLN		258	54.771	86.519	2.876	0.35	31.23
3635		AGLN		258	55.724				
3636		BGLN		258		84.264	2.547	0.65	32.97
		AGLN			55.645	86.639 83.279	2.016	0.35	30.93
3637		BGLN		258	54.977		2.618	0.65	32.08
3638		AGLN		258	53.503	86.266	2.585	0.35	30.18
3639	C			258	56.103	84.792	1.389	0.65	33.37
3644		GLN		258	55.203	85.967	7.400	1.00	32.82
3645	0	GLN		258	55.460	87.123	7.720	1.00	33.46
3646	N	GLN		259	54.266	85.249	8.000	1.00	33.70
3648	CA	GLN		259	53.452	85.780	9.084	1.00	
3650	CB	GLN		259	52.395	84.756	9.463	1.00	35.35
3653	CG	GLN		259	51.346	85.257	10.436	1.00	38.57
3656	CD	GLN		259	50.161	84.331	10.482	1.00	42.61
3657	OE1	GLN		259	49.161	84.555	9.787	1.00	45.33
3658	NE2	GLN		259	50.272	83.263	11.278	1.00	44.63
3661	C	GLN		259	54.281	86.173	10.320	1.00	34.20
3662	0	GLN		259	53.948	87.154	10.990	1.00	33.93
3663	N	LEU	Α	260	55.347	85.419	10.613	1.00	33.21
3665	CA	LEU	Α	260	56.247	85.737	11.734	1.00	32.74
3667	CB	LEU	Α	260	56.676	84.463	12.474	1.00	32.73
3670	CG	LEU	Α	260	55.629	83.549	13.112	1.00	34.09
3672	CD1	LEU	A	260	56.300	82.734	14.206	1.00	35.07
3676	CD2	LEU	Α	260	54.412	84.295	13.676	1.00	35.20
3680	C	LEU	Α	260	57.514	86.495	11.326	1.00	31.74
3681	0	LEU	Α	260	58.348	86.790	12.172	1.00	31.90
3682	N	GLY	Α	261	57.670	86.808	10.043	1.00	30.66
3684	CA	GLY	Α	261	58.858	87.495	9.565	1.00	29.51
3687	C	GLY	Α	261	60.157	86.732	9.759	1.00	28.74
3688	0	GLY	Α	261	61.198	87.333	9.998	1.00	28.52
3689	N	LYS	Α	262	60.099	85.405	9.649	1.00	27.62
3691	CA	LYS	Α	262	61.296	84.575	9.707	1.00	26.77
3693	CB	LYS	Α	262	60.934	83.092	9.572	1.00	26.29
3696	CG	LYS	Α	262	60.021	82.536	10.642	1.00	25.90
3699	CD	LYS	Α	262	60.797	82.141	11.884	1.00	26.17
3702	CE	LYS	Α	262	59.882	81.593	12.965	1.00	26.68
3705	NZ	LYS	Α	262	60.644	81.319	14.214	1.00	
3709	C	LYS	Α	262	62.280	84.943	8.595		26.39
3710	0	LYS	Α	262	61.884	85.161	7.445		26.03
3711	N	SER	Α	263	63.563	85.005	8.943		26.23
3713	CA	SER	Α	263	64.629	85.019	7.944		26.10
3715	CB	SER		263	65.975	85.311	8.586		26.43
3718	OG	SER		263	65.979	86.581	9.207	1.00	
3720	С	SER		263	64.666	83.652	7.247	1.00	
3721	0	SER		263	64.899	82.629	7.898	1.00	
3722	N	THR		264	64.388	83.642	5.942	1.00	
3724	CA	THR		264	64.408	82.408	5.149		25.89
3726	СВ	THR		264	62.975	81.922	4.812		26.14
3728	OG1	THR		264	62.368	82.789	3.847		26.91

FIGURE 3 (Cont.) BK

A	В	С	D	E	F	G	Н	I	J
3730	CG2	THR	Δ	264	62.046	81.992	6.033	1 00	26.45
3734	C	THR		264	65.189	82.591	3.856		25.77
3735	0	THR		264	65.538	83.722	3.472	1.00	25.77
3736	N	TYR		265	65.479	81.471	3.195	1.00	
3738	CA	TYR		265	66.114	81.507		1.00	25.31
3740	CB	TYR		265	66.555		1.886		
3743	CG	TYR		265		80.104	1.428		24.84
3744	CD1	TYR			67.953	79.767	1.902		24.29
	CE1			265	69.012	79.698	1.010	1.00	23.63
3746 3748	CZ	TYR TYR		265	70.282 70.545	79.407	1.423	1.00	24.04
3749		TYR		265		79.200	2.759	1.00	24.29
	OH			265	71.827	78.928	3.168		24.41
3751	CE2	TYR		265	69.521	79.276	3.685		24.92
3753	CD2	TYR		265	68.225	79.566	3.250		23.77
3755	C	TYR		265	65.240	82.222	0.843	1.00	25.25
3756	0	TYR		265	65.717	83.149	0.211	1.00	25.83
3757	N	PRO		266	63.982	81.823	0.658	1.00	25.61
3758	CA	PRO		266	63.108	82.515	-0.307	1.00	
3760	CB	PRO		266	61.812	81.700	-0.284	1.00	
3763	CG	PRO		266	61.876	80.854	0.923	1.00	26.04
3766	CD	PRO		266	63.311	80.683	1.293	1.00	25.37
3769	C	PRO		266	62.825	83.980	0.027	1.00	25.95
3770	0	PRO		266	62.702	84.784	-0.900		25.00
3771	N	ALA		267	62.738	84.326	1.311		26.04
3773	CA	ALA		267	62.503	85.719	1.697	1.00	26.33
3775	CB	ALA		267	62.193	85.853	3.166	1.00	26.37
3779	C	ALA		267	63.694	86.578	1.309	1.00	26.47
3780	0	ALA		267	63.512	87.637	0.734	1.00	26.90
3781	N	LEU		268	64.906	86.094	1.574	1.00	26.35
3783	CA	LEU		268	66.124	86.814	1.213	1.00	26.27
3785	CB	LEU		268	67.337	86.201	1.924	1.00	26.30
3788	CG	LEU		268	68.691	86.873	1.690	1.00	27.65
3790	CD1	LEU		268	68.728	88.322	2.211		28.07
3794	CD2	LEU		268	69.803	86.053	2.316	1.00	28.26
3798	С	LEU		268	66.386	86.828	-0.294	1.00	26.01
3799	0	LEU	Α	268	66.541	87.899	-0.898	1.00	25.44
3800	N	LEU		269	66.439	85.633	-0.881	1.00	25.58
3802	CA	LEU		269	66.963	85.430	-2.234	1.00	25.43
3804	CB	LEU		269	67.755	84.113	-2.298		25.44
3807	CG	LEU		269	68.906	83.896	-1.320		26.67
3809	CD1			269	69.520	82.486	-1.510	1.00	25.96
3813		LEU		269	69.960	84.976	-1.479		27.24
3817	C	LEU		269	65.902	85.380	-3.316		24.91
3818	0	LEU		269	66.226	85.454	-4.490	1.00	24.92
3819	N	GLY		270	64.640	85.253	-2.933		24.87
3821	CA	GLY		270	63.584	84.945	-3.884		24.94
3824	С	GLY		270	63.529	83.446	-4.151		25.33
3825	0	GLY		270	64.488	82.724	-3.871		25.08
3826	N	LEU		271	62.415	82.985	-4.699		25.79
3828	CA	LEU		271	62.170	81.567	-4.899		26.67
3830	CB	LEU		271	60.732	81.320	-5.383		27.35
3833	CG	LEU		271	59.602	81.477	-4.365		28.42
3835	CD1	LEU	A	271	58.252	81.403	-5.068	1.00	29.93

FIGURE 3 (Cont.)BL

Α	В	С	D	E	F		G	H		I		J
			_					_				
3839	CD2	LEU		271	59.687		.413	-3.:				28.63
3843	C	LEU		271	63.162		.914	-5.				27.13
3844	0	LEU		271	63.593		796	-5.				27.11
3845	N	GLU		272	63.536		599	-6.				27.48
3847	CA	GLU		272	64.429		018	-7.				28.05
3849	CB	GLU		272	64.488		. 905	-9.		1.0		28.98
3852	CG	GLU		272	65.687		611	-10.				31.69
3855	CD	GLU		272	65.592		. 253	-11.				35.38
3856		GLU		272	66.103		648	-12.4				39.00
3857		GLU		272	65.013		.354			1.0		37.35
3858	C	GLU		272	65.850		.739	-7.		1.0		27.43
3859	0	GLU		272	66.427		.668	-7.				27.14
3860	N	GLN		273	66.432		697	-6.				26.16
3862	CA	GLN		273	67.799		.563	-6.				26.17
3864	CB	GLN		273	68.364		.909	-5.				26.14
3867 3870	CG CD	GLN GLN		273 273	68.642		.881	-6.		1.0		29.26
3871		GLN		273	69.025		.266	-6.4		1.0		32.23
3872	NE2	GLN			69.828		.405	-5.4		1.0		34.54
3875	C	GLN		273 273	68.464		. 295	-7.		1.0		34.59
3876	0				67.854 68.856		.566	-5.				25.40
3877	N	GLN ALA		273 274	66.776		905	-4.				25.15
3879	CA	ALA		274	66.681		.485 .514	-4.: -3.:				25.33
3881	CB	ALA		274	65.429		7.514	-2.4				25.32
3885	C	ALA		274	66.665		1.097	-3.				25.59 25.68
3886	0	ALA		274	67.388		.213	-3.				
3887	N	ARG		275	65.860		.213	-4.		1.0		25.35 25.78
3889	CA	ARG		275	65.753		.631	-5.				26.49
3891	СВ	ARG		275	64.725		.697	-6.0				26.59
3894	CG	ARG		275	63.311		.604	-6.				27.19
3897	CD	ARG		275	62.284		.791	-7.				29.91
3900	NE	ARG		275	60.926		.575	-6.				31.85
3902	CZ	ARG		275	59.886		.379	-7.0		1.0		34.22
3903	NH1	ARG		275	59.998		.504	-7.		1.0		35.16
3906	NH2	ARG		275	58.706		.047	-6.4				35.99
3909	С	ARG		275	67.091		.201	-6.3		1.0		26.94
3910	0	ARG	Α	275	67.468		.039	-5.5		1.0		27.03
3911	N	LYS	Α	276	67.816		.155	-6.0				27.58
3913	CA	LYS		276	69.145		.929	-7.2				28.35
3915	CB	LYS	Α	276	69.641		.193	-7.5				29.25
3918	CG	LYS	Α	276	71.101		.163	-8.4				31.10
3921	CD	LYS		276	71.288		.283	-9.0	637			34.04
3924	CE	LYS	Α	276	72.514		.689	-10.4				35.05
3927	NZ	LYS	Α	276	73.803	77	.493	-9.	748			35.48
3931	C	LYS	Α	276	70.130	76	.552	-6.3	132	1.0	0	28.37
3932	0	LYS	Α	276	70.987	75	.692	-6.3		1.0	0	28.80
3933	N	LYS	Α	277	70.054	77	.222	-4.5		1.0	0	28.08
3935	CA	LYS	Α	277	70.938	76	.890	-3.8	873	1.0	0	27.92
3937	CB	LYS		277	70.723		.824	-2.6	675			28.22
3940	CG	LYS		277	71.163	79	.279	-2.9	921	1.0	0	30.08
3943	CD	LYS		277	72.546		.581	-2.3				31.98
3946	CE	LYS	Α	277	72.871	81	.085	-2.4	114	1.0	0	32.86

FIGURE 3 (Cont.)BM

3949 NZ LYS A 277 70.680 75.438 -3.453 1.00 27.24 3953 C LYS A 277 70.680 75.438 -3.453 1.00 26.72 3955 N ALA A 278 69.411 75.041 -3.393 1.00 26.71 3957 CA ALA A 278 69.553 73.682 -2.2960 1.00 26.99 3965 C ALA A 278 69.589 72.551 -3.949 1.00 27.61 3965 N ARG 279 69.427 72.948 -5.234 1.00 27.61 3965 N ARG 279 69.427 72.948 -5.234 1.00 28.16 3969 CZ ARG 279 69.910 71.996 -8.886 1.00 32.19 3972 CG ARG 279 69.910 71.996 -8.886 1.00	A	В	С	D	E	F	G	Н	I	J
3953 C LYS A 277 70.680 75.438 -3.453 1.00 27.24 3955 N ALA A 278 69.411 75.041 -3.393 1.00 26.79 3955 CA ALA A 278 69.053 73.682 -2.960 1.00 26.99 3953 C ALA A 278 69.589 72.651 -3.949 1.00 27.26 3963 C ALA A 279 69.589 72.613 -3.566 1.00 27.66 3965 N ARG 279 69.869 72.070 -6.311 1.00 28.87 3967 CA ARG 279 69.332 72.603 -7.641 1.00 28.87 3975 CD ARG 279 69.160 72.414 -10.158 1.00 35.33 3976 CD ARG 279 68.039 73.319 -9.815 1.00	3949	NZ	LYS	Α	277	74.277	81.323	-2.846	1.00	33.80
3954 O LYS A 277 71.620 74.699 -3.201 1.00 26.52 3957 CA ALA A 278 69.453 73.682 -2.960 1.00 26.71 3957 CA ALA A 278 69.553 73.682 -2.960 1.00 26.84 3963 C ALA A 278 69.589 72.651 -3.949 1.00 26.69 3965 N ARG A 279 69.869 72.670 -6.311 1.00 28.16 3967 CA ARG A 279 69.869 72.070 -6.311 1.00 28.16 3975 CD ARG A 279 69.910 71.996 -8.886 1.00 35.33 3978 NE ARG A 279 69.027 75.256 -10.711 1.00 38.00 3981 NH1 ARG A 279 68.039 73.319 -9.815 1.00 38.95 3984 NH2<										
3955 N ALA A 278 69.411 75.041 -3.393 1.00 26.71 3957 CA ALA A 278 69.053 73.5662 -2.960 1.00 26.98 3963 C ALA A 278 69.589 72.651 -3.949 1.00 27.26 3964 O ALA A 278 69.589 72.651 -3.949 1.00 27.26 3965 N ARG A 279 69.869 72.070 -6.311 1.00 28.16 3969 CB ARG A 279 69.910 71.996 -8.866 1.00 22.16 3975 CD ARG A 279 69.910 71.996 -8.866 1.00 35.33 3978 NE ARG A 279 69.160 72.414 -10.158 1.00 35.33 3980 CZ ARG A 279 69.027 75.256 -10.711 1.00 40.27 3984 NHI<										
3957 CA ALA A 278 69.053 73.662 -2.960 1.00 26.84 3963 C ALA A 278 67.544 73.546 -2.823 1.00 26.84 3964 O ALA A 278 70.141 71.636 -3.566 1.00 26.69 3965 N ARG A 279 69.427 72.948 -5.234 1.00 22.61 3969 CB ARG A 279 69.869 72.070 -6.311 1.00 28.87 3972 CG ARG A 279 69.910 71.996 -8.886 1.00 32.19 3975 CD ARG A 279 69.160 72.414 -10.158 1.00 38.00 3981 NH1 ARG A 279 68.039 73.319 -9.815 1.00 38.95 3984 NH2 ARG A 279 71.889 71.923 -6.336 1.00 22.24 3988 O </td <td></td>										
3959 CB ALA A 278 67.544 73.546 -2.823 1.00 26.84 3963 C ALA A 278 69.589 72.651 -3.949 1.00 27.26 3965 N ARG A 279 69.427 72.948 -5.234 1.00 27.61 3967 CA ARG A 279 69.869 72.070 -6.311 1.00 28.16 3975 CB ARG A 279 69.910 71.996 -8.886 1.00 32.19 3975 CD ARG A 279 69.910 71.996 -8.886 1.00 35.33 3978 NE ARG A 279 68.039 73.319 -9.815 1.00 38.95 3981 NH1 ARG A 279 69.027 75.256 -10.711 1.00 40.27 3987 C ARG A 279 71.389 71.923 -6.512 1.00 26.39 3987 C <td></td>										
3963 C ALA A 278 69.589 72.651 -3.949 1.00 27.26 3965 N ARG A 279 69.427 72.948 -5.234 1.00 27.66 3967 CA ARG A 279 69.869 72.070 -6.311 1.00 28.16 3969 CB ARG A 279 69.322 72.603 -7.641 1.00 28.87 3975 CD ARG A 279 69.910 71.996 -8.886 1.00 32.19 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.90 3981 NH1 ARG A 279 66.924 75.256 -10.711 1.00 40.27 3987 C ARG A 279 66.924 75.329 -9.815 1.00 27.02 3988 N ASP A 280 72.16 73.021 -6.128 1.00 25.90 3993 CB <td></td>										
3964 O ALA A 278 70.141 71.636 -3.566 1.00 26.94 3965 NA ARG A 279 69.427 72.948 -5.234 1.00 27.61 3969 CA ARG A 279 69.869 72.070 -6.311 1.00 28.87 3972 CG ARG A 279 69.910 71.996 -8.886 1.00 32.19 3975 CD ARG A 279 69.160 72.414 -10.158 1.00 38.00 3981 NH ARG A 279 66.029 73.319 -9.871 1.00 38.95 3981 NH ARG A 279 66.924 75.256 -10.711 1.00 40.27 3984 NE ARG A 279 71.389 71.923 -6.512 1.00 27.02 3987 C ARG A 279 71.885 70.819 -6.512 1.00 27.02 3989 N A		С								
3965 N ARG A 279 69.427 72.948 -5.234 1.00 27.61 3967 CA ARG A 279 69.869 72.070 -6.311 1.00 28.16 3972 CG ARG A 279 69.910 71.996 -8.886 1.00 32.19 3975 CD ARG A 279 69.910 72.414 -10.158 1.00 35.33 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.03 3981 NH1 ARG A 279 68.039 73.526 -10.711 1.00 40.27 3984 NH1 ARG A 279 66.924 75.256 -10.711 1.00 40.27 3987 C ARG A 279 71.885 70.819 -6.512 1.00 26.38 3988 C ARG A 279 71.885										
3967 CA ARG A 279 69.869 72.070 -6.311 1.00 28.16 3969 CB ARG A 279 69.332 72.603 -7.641 1.00 28.87 3975 CD ARG A 279 69.160 72.414 -10.158 1.00 35.33 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.00 3980 CZ ARG A 279 68.005 74.632 -10.133 1.00 38.95 3981 NH1 ARG A 279 66.924 75.329 -9.815 1.00 27.24 3984 NH2 ARG A 279 71.885 70.819 -6.336 1.00 27.02 3988 O ARG A 279 71.885 70.21 -6.122 1.00 27.02 3989 N ASP A 280 73.586 72.995 -6.052 1.00 26.33 3991 CB	3965	N								
3969 CB ARG A 279 69.332 72.603 -7.641 1.00 28.87 3975 CD ARG A 279 69.910 71.996 -8.886 1.00 35.33 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.00 3981 NH1 ARG A 279 66.005 74.632 -10.133 1.00 38.95 3981 NH1 ARG A 279 66.924 75.329 -9.815 1.00 38.95 3987 C ARG A 279 71.389 71.923 -6.336 1.00 27.24 3988 O ARG A 279 71.389 71.923 -6.336 1.00 27.24 3989 N ASP A 280 72.166 73.786 72.995 -6.059 1.00 26.36 3991 CA ASP A 280 </td <td></td> <td>CA</td> <td></td> <td></td> <td>279</td> <td></td> <td></td> <td></td> <td></td> <td></td>		CA			279					
3972 CG ARG A 279 69.910 71.996 -8.886 1.00 32.19 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 35.33 3980 CZ ARG A 279 68.035 73.319 -9.871 1.00 38.95 3981 NH1 ARG A 279 66.027 75.256 -10.711 1.00 40.27 3984 NH2 ARG A 279 66.924 75.329 -9.815 1.00 27.24 3988 O ARG A 279 71.885 70.819 -6.512 1.00 27.02 3988 O ARG A 279 71.885 70.819 -6.512 1.00 26.36 3991 CA ASP A 280 72.116 73.021 -6.128 1.00 26.39 3993 CB ASP A 280 74.006<	3969	CB	ARG	Α						
3975 CD ARG A 279 69.160 72.414 -10.158 1.00 35.33 3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.05 3981 NH1 ARG A 279 69.027 75.256 -10.711 1.00 40.27 3984 NH2 ARG A 279 66.924 75.329 -9.815 1.00 38.71 3987 C ARG A 279 71.389 71.923 -6.316 1.00 27.24 3988 O ARG A 279 71.885 70.819 -6.5122 1.00 27.02 3988 O ARG A 279 71.885 70.819 -6.5122 1.00 26.36 3991 CA ASP A 280 73.586 72.995 -6.059 1.00 26.36 3991 CA ASP A 280 74.09										
3978 NE ARG A 279 68.039 73.319 -9.871 1.00 38.00 3980 CZ ARG A 279 68.005 74.632 -10.133 1.00 38.95 3981 NH1 ARG A 279 66.924 75.329 -9.815 1.00 38.71 3987 C ARG A 279 71.389 71.923 -6.336 1.00 27.24 3988 O ARG A 279 71.389 71.923 -6.336 1.00 27.24 3989 N ASP A 280 72.116 73.021 -6.128 1.00 26.36 3991 CA ASP A 280 74.150 74.420 -6.055 1.00 26.39 3996 CG ASP A 280 74.090 76.423 -7.315 1.00 28.33 3997 CD ASP A 280 74.090 <td></td> <td>CD</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>		CD								
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4037 C ILE A 282 73.241 67.719 -4.788 1.00 26.42 4038 O ILE A 282 73.728 66.602 -4.641 1.00 26.98 4039 N ASP A 283 73.571 68.511 -5.802 1.00 27.38 4041 CA ASP A 283 74.607 68.111 -6.753 1.00 28.16 4043 CB ASP A 283 74.799 69.165 -7.851 1.00 28.99 4046 CG ASP A 283 73.578 69.319 -8.758 1.00 31.72 4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.48 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48 <td>4033</td> <td>CG2</td> <td>ILE</td> <td>Α</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	4033	CG2	ILE	Α						
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4039 N ASP A 283 73.571 68.511 -5.802 1.00 27.38 4041 CA ASP A 283 74.607 68.111 -6.753 1.00 28.16 4043 CB ASP A 283 74.799 69.165 -7.851 1.00 28.99 4046 CG ASP A 283 73.578 69.319 -8.758 1.00 31.72 4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.48 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4038	0	ILE	Α	282					
4041 CA ASP A 283 74.607 68.111 -6.753 1.00 28.16 4043 CB ASP A 283 74.799 69.165 -7.851 1.00 28.99 4046 CG ASP A 283 73.578 69.319 -8.758 1.00 31.72 4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.48 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4039	N	ASP	Α	283	73.571				
4043 CB ASP A 283 74.799 69.165 -7.851 1.00 28.99 4046 CG ASP A 283 73.578 69.319 -8.758 1.00 31.72 4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.48 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4041	CA	ASP	Α	283	74.607	68.111	-6.753		
4046 CG ASP A 283 73.578 69.319 -8.758 1.00 31.72 4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.86 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4043	CB	ASP	Α	283				1.00	
4047 OD1 ASP A 283 73.510 70.341 -9.477 1.00 36.96 4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.86 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4046	CG	ASP	Α	283					
4048 OD2 ASP A 283 72.644 68.493 -8.830 1.00 35.17 4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.86 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4047	OD1	ASP	Α			70.341	-9.477		
4049 C ASP A 283 75.929 67.903 -5.997 1.00 27.86 4050 O ASP A 283 76.696 67.003 -6.319 1.00 27.48	4048	OD2	ASP	Α	283		68.493			
	4049	С			283	75.929	67.903			
4051 N ASP A 284 76.189 68.740 -4.988 1.00 27.56	4050	0	ASP	Α	283	76.696	67.003	-6.319	1.00	27.48
	4051	N	ASP	Α	284	76.189	68.740	-4.988	1.00	27.56

FIGURE 3 (Cont.)BN

Α	В	С	D	E	F	G	Н	I	J
4053	CA	ASP	A	284	77.405	68.623	-4.177	1.00	27.43
4055	CB	ASP		284	77.573	69.869	-3.296	1.00	27.98
4058	CG	ASP	Α	284	78.753	69.774	-2.351	1.00	29.55
4059	OD1	ASP	A	284	79.871	70.166	-2.754	1.00	34.48
4060	OD2	ASP	Α	284	78.662	69.347	-1.179	1.00	30.96
4061	C	ASP	Α	284	77.344	67.351	-3.320	1.00	26.91
4062	0	ASP	Α	284	78.347	66.666	-3.137	1.00	26.70
4063	N	ALA	Α	285	76.154	67.039	-2.817	1.00	26.35
4065	CA	ALA	Α	285	75.935	65.830	-2.041	1.00	26.26
4067	CB	ALA	Α	285	74.514	65.811	-1.452	1.00	26.18
4071	C	ALA	Α	285	76.164	64.607	-2.913	1.00	26.41
4072	0	ALA	Α	285	76.774	63.648	-2.469	1.00	26.46
4073	N	ARG		286	75.687	64.647	-4.156	1.00	26.93
4075	CA	ARG		286	75.888	63.543	-5.095	1.00	27.77
4077	CB	ARG		286	75.153	63.778	-6.413	1.00	28.06
4080	CG	ARG		286	73.650	63.500	-6.353	1.00	30.42
4083	CD	ARG		286	72.949	63.511	-7.727	1.00	33.16
4086	NE	ARG		286	71.739	62.694	-7.695	1.00	35.04
4088	CZ	ARG		286	71.709	61.365	-7.828	1.00	37.56
4089	NH1	ARG		286	72.820	60.653	-8.041	1.00	37.77
4092	NH2	ARG		286	70.544	60.731	-7.757	1.00	37.95
4095	C	ARG		286	77.377	63.333	-5.364	1.00	28.02
4096	0	ARG		286	77.837	62.202	-5.438	1.00	27.64
4097	N	GLN		287	78.120	64.427	-5.478	1.00	28.41
4099	CA	GLN		287	79.550	64.352	-5.768	1.00	29.05
4101	CB	GLN		287	80.163	65.742	-5.984	1.00	29.26
4104 4107	CG CD	GLN GLN		287	79.870	66.348	-7.343	1.00	31.16
4107	OE1	GLN		287 287	80.342 81.544	65.469 65.280	-8.494 -8.687	1.00	34.10 36.57
4109	NE2	GLN		287	79.396	64.921	-9.248	1.00	34.65
4112	C	GLN		287	80.260	63.638	-4.645	1.00	28.84
4113	Ö	GLN		287	81.060	62.747	-4.898	1.00	29.43
4114	N	SER		288	79.946	64.002	-3.403	1.00	28.72
4116	CA	SER		288	80.514	63.331	-2.234	1.00	28.70
4118	CB	SER		288	79.948	63.912	-0.930	1.00	28.50
4121	OG	SER		288	80.451	65.214	-0.693	1.00	28.19
4123	С	SER	Α	288	80.254	61.824	-2.255	1.00	28.86
4124	0	SER	Α	288	81.143	61.046	-1.948	1.00	28.79
4125	N	LEU	Α	289	79.028	61.428	-2.579		29.44
4127	CA	LEU	Α	289	78.666	60.005	-2.650	1.00	29.79
4129	CB	LEU	Α	289	77.163	59.818	-2.910	1.00	29.50
4132	CG	LEU	Α	289	76.184	60.273	-1.815	1.00	28.59
4134	CD1	LEU	Α	289	74.747	60.026	-2.249	1.00	28.94
4138		LEU	Α	289	76.473	59.585	-0.493	1.00	27.92
4142	C	LEU		289	79.472	59.246	-3.717	1.00	30.81
4143	0	LEU		289	79.732	58.062	÷3.545		30.71
4144	N	LYS		290	79.870	59.919	-4.800		31.59
4146	CA	LYS		290	80.704	59.288	-5.837		32.26
4148	CB	LYS		290	80.998	60.268	-6.989		32.55
4151	CG	LYS		290	79.794	60.560	-7.898		34.13
4154	CD	LYS		290	80.188	61.386	-9.153		35.23
4157	CE	LYS	A	290	79.129	61.238	-10.259	1.00	36.81

FIGURE 3 (Cont.)BO

A	В	С	D	E	F	G	H	I	J
47.50		* ***				<i></i>			
4160	NZ	LYS		290	79.083	62.387	-11.229	1.00	37.86
4164	C	LYS		290	82.012	58.741	-5.256	1.00	32.60
4165	0	LYS		290	82.471	57.679	-5.650	1.00	33.03
4166	N	GLN		291	82.589	59.462	-4.300	1.00	33.38
4168	CA	GLN		291	83.796	59.026	-3.599	1.00	34.01
4170	CB	GLN		291	84.253	60.103	-2.607	1.00	34.60
4173	CG	GLN		291	84.614	61.448	-3.230	1.00	35.87
4176	CD	GLN		291	85.108	62.446	-2.197	1.00	37.47
4177	OE1	GLN		291	86.039	62.155	-1.446	1.00	39.36
4178	NE2	GLN		291	84.483	63.615	-2.149	1.00	39.06
4181	С	GLN		291	83.589	57.715	-2.830	1.00	34.18
4182	0	GLN		291	84.513	56.909	-2.707	1.00	34.15
4183	N	LEU	Α	292	82.385	57.520	-2.294	1.00	33.99
4185	CA	LEU	Α	292	82.047	56.287	-1.591	1.00	34.26
4187	CB	LEU	Α	292	80.849	56.509	-0.670	1.00	33.95
4190	CG	LEU	A	292	81.061	57.578	0.398	1.00	33.40
4192	CD1	LEU	Α	292	79.805	57.720	1.223	1.00	33.09
4196	CD2	LEU	Α	292	82.269	57.242	1.274	1.00	33.91
4200	C	LEU	Α	292	81.738	55.137	-2.533	1.00	34.79
4201	0	LEU	Α	292	82.073	53.989	-2.239	1.00	34.64
4202	N	ALA	Α	293	81.072	55.445	-3.642	1.00	35.56
4204	CA	ALA	Α	293	80.741	54.450	-4.660	1.00	36.49
4206	CB	ALA	Α	293	79.825	55.061	-5.712	1.00	36.38
4210	С	ALA	Α	293	82.012	53.886	-5.311	1.00	37.32
4211	0	ALA	Α	293	82.015	52.758	-5.799	1.00	37.70
4212	N	GLU	Α	294	83.075	54.690	-5.296	1.00	38.52
4214	CA	GLU	Α	294	84.421	54.297	-5.744	1.00	39.54
4216	CB	GLU	Α	294	85.353	55.513	-5.677	1.00	39.78
4219	CG	GLU	Α	294	86.404	55.572	-6.767	1.00	41.97
4222	CD	GLU	Α	294	86.407	56.897	-7.488	1.00	43.76
4223	OE1	GLU	Α	294	86.681	57.915	-6.825	1.00	46.66
4224	OE2	GLU	Α	294	86.129	56.921	-8.705	1.00	45.53
4225	С	GLU	Α	294	85.034	53.179	-4.895	1.00	39.49
4226	0	GLU	Α	294	85.883	52.422	-5.363	1.00	40.00
4227	N	GLN	Α	295	84.617	53.112	-3.638	1.00	39.43
4229	CA	GLN	Α	295	85.085	52.109	-2.700	1.00	39.30
4231	CB	GLN	Α	295	85.306	52.752	-1.324	1.00	39.51
4234	CG	GLN	Α	295	86.094	54.061	-1.348	1.00	40.85
4237	CD	GLN	Α	295	86.003	54.825	-0.033	1.00	42.68
4238	OE1	GLN	Α	295	85.958	54.217	1.037	1.00	44.83
4239	NE2	GLN	Α	295	85.983	56.156	-0.110	1.00	42.30
4242	С	GLN	Α	295	84.087	50.944	-2.594	1.00	38.62
4243	0	GLN	Α	295	84.083	50.210	-1.605	1.00	38.99
4244	N	SER	Α	296	83.250	50.794	-3.616	1.00	37.61
4246	CA	SER	Α	296	82.260	49.718	-3.721	1.00	36.98
4248	CB	SER	A	296	82.963	48.362	-3.884	1.00	37.17
4251	OG	SER	Α	296	83.487	48.241	-5.197	1.00	38.77
4253	С	SER	Α	296	81.210	49.685	-2.598	1.00	35.68
4254	0	SER	Α	296	80.722	48.617	-2.206	1.00	35.55
4255	N	LEU		297	80.867	50.865	-2.092	1.00	34.25
4257	CA	LEU	Α	297	79.710	51.032	-1.218	1.00	32.88
4259	CB	LEU	A	297	79.997	52.090	-0.161	1.00	32.92

FIGURE 3 (Cont.) BP

A	В	С	D	E	F	G	H	I	J
4262	CG	LEU		297	81.178		0.755	1.00	33.21
4264	CD1	LEU		297	81.567		1.532	1.00	
4268	CD2	LEU		297	80.872		1.704	1.00	
4272	C	LEU		297	78.507		-2.074		31.66
4273	0	LEU		297	78.621		-2.988		31.32
4274	N	ASP		298	77.361		-1.799	1.00	30.63
4276	CA	ASP		298	76.127		-2.528		29.60
4278	CB	ASP		298	75.150		-2.371		29.83
4281	CG	ASP		298	73.911		-3.251	1.00	30.98
4282	OD1	ASP		298	73.673		-3.843	1.00	30.78
4283		ASP		298	73.117		-3.407	1.00	32.78
4284	С	ASP		298	75.516		-2.021		28.62
4285	0	ASP		298	74.919		-0.953		27.93
4286	N	THR		299	75.655		-2.801	1.00	27.78
4288	CA	THR		299	75.152		-2.395		27.48
4290	CB	THR		299	76.121		-2.850	1.00	27.79
4292	OG1	THR		299	76.198	55.923	-4.282	1.00	27.64
4294	CG2	THR		299	77.522		-2.397	1.00	27.86
4298	С	THR	Α	299	73.775		-2.963	1.00	26.98
4299	0	THR	A	299	73.314	56.269	-2.852		26.90
4300	N	SER	Α	300	73.115	54.136	-3.549	1.00	25.87
4302	CA	SER	Α	300	71.884	54.371	-4.303	1.00	25.78
4304	CB	SER	Α	300	71.469	53.116	-5.083	1.00	25.66
4307	OG	SER	Α	300	71.181	52.042	-4.210	1.00	28.03
4309	С	SER	Α	300	70.718	54.922	-3.460	1.00	24.86
4310	0	SER	Α	300	69.989	55.799	-3.922	1.00	24.04
4311	N	ALA	Α	301	70.538	54.423	-2.237	1.00	24.31
4313	CA	ALA	Α	301	69.491	54.957	-1.356	1.00	23.85
4315	CB	ALA	Α	301	69.266	54.058	-0.138	1.00	23.74
4319	C	ALA	Α	301	69.813	56.402	-0.925	1.00	23.51
4320	0	ALA	Α	301	68.927	57.234	-0.865	1.00	22.49
4321	N	LEU	A	302	71.082	56.696	-0.670	1.00	23.59
4323	CA	LEU	Α	302	71.476	58.050	-0.254	1.00	24.04
4325	CB	LEU	Α	302	72.893	58.059	0.321	1.00	23.68
4328	CG	LEU	Α	302	73.047	57.380	1.677	1.00	24.07
4330	CD1	LEU	Α	302	74.495	57.511	2.165	1.00	25.59
4334	CD2	LEU	Α	302	72.085	57.972	2.680	1.00	24.26
4338	C	LEU	Α	302	71.375	59.070	-1.370	1.00	24.05
4339	0	LEU		302	71.128	60.238	-1.104	1.00	24.30
4340	N	GLU	Α	303	71.575	58.648	-2.614	1.00	24.92
4342	CA	GLU	Α	303	71.455	59.578	-3.734	1.00	25.79
4344	СВ	GLU	Α	303	72.238	59.158	-4.988	1.00	26.38
4347	CG	GLU	A	303	72.152	57.732	-5.448	1.00	28.99
4350	CD	GLU	Α	303	73.344	57.345	-6.333	1.00	31.29
4351	OE1	GLU	Α	303	73.673	58.127	-7.247	1.00	31.21
4352	OE2	GLU	Α	303	73.966		-6.098	1.00	33.39
4353	С	GLU	Α	303	69.982	59.834	-4.045	1.00	25.52
4354	0	GLU	Α	303	69.605	60.961	-4.347	1.00	25.13
4355	N	ALA	Α	304	69.152	58.797	-3.927	1.00	25.73
4357	CA	ALA		304	67.709	58.953	-4.149	1.00	25.33
4359	CB	ALA		304	67.020	57.609	-4.201	1.00	25.75
4363	С	ALA	Α	304	67.099	59.830	-3.059	1.00	25.32

FIGURE 3 (Cont.)BQ

A	В	С	D	E	F	G	Н	I	J
4364	0	ALA	Α	304	66.202	60.633	-3.328	1.00	24.76
4365	N	LEU		305	67.591	59.677	-1.828	1.00	
4367	CA	LEU	Α	305	67.117	60.499	-0.711	1.00	25.23
4369	CB	LEU	Α	305	67.707	59.988	0.608	1.00	25.28
4372	CG	LEU	A	305	67.209	60.548	1.945	1.00	27.23
4374	CD1	LEU	Α	305	67.788	61.919	2.199	1.00	29.43
4378	CD2	LEU	Α	305	65.687	60.595	2.012	1.00	28.69
4382	С	LEU	Α	305	67.520	61.954	-0.959	1.00	24.32
4383	0	LEU	Α	305	66.719	62.872	-0.780	1.00	23.70
4384	N	ALA	A	306	68.758	62.146	-1.399	1.00	23.80
4386	CA	ALA	Α	306	69.282	63.481	-1.672	1.00	24.14
4388	CB	ALA	Α	306	70.733	63.405	-2.153	1.00	24.17
4392	С	ALA	Α	306	68.410	64.218	-2.687	1.00	24.07
4393	0	ALA		306	68.063	65.382	-2.480	1.00	
4394	N	ASP		307	68.027	63.538	-3.761	1.00	24.24
4396	CA	ASP		307	67.146	64.143	-4.772	1.00	24.99
4398	CB	ASP		307	67.015	63.231	-5.990	1.00	25.46
4401	CG	ASP		307	68.259	63.225	-6.840	1.00	27.73
4402	OD1	ASP		307	68.311	62.445	-7.819	1.00	32.11
4403	OD2	ASP		307	69.231	63.968	-6.614	1.00	30.06
4404	C	ASP		307	65.751	64.427	-4.242	1.00	24.15
4405	0	ASP		307	65.146	65.464	-4.565	1.00	23.53
4406	N	TYR		308	65.233	63.497	-3.445	1.00	23.64
4408	CA	TYR		308	63.890	63.636	-2.889	1.00	23.49
4410	CB	TYR		308	63.465	62.369	-2.150	1.00	23.53
4413	CG	TYR		308	62.066	62.432	-1.543	1.00	23.83
4414	CD1	TYR		308	61.882	62.358	-0.171		24.83
4416	CE1	TYR		308	60.607	62.425	0.392	1.00	25.12
4418 4419	CZ OH	TYR TYR		308 308	59.501	62.553	-0.424	1.00	26.00
4421	CE2	TYR		308	58.239	62.602	0.134	1.00	26.70
4423	CD2	TYR		308	59.660 60.939	62.622 62.568	-1.798 -2.344	1.00	25.30
4425	C	TYR		308	63.824	64.844	-1.957	1.00	23.99 23.57
4426	ō	TYR		308	62.829	65.529	-1.919	1.00	22.72
4427	N	ILE		309	64.902	65.112	-1.229	1.00	24.12
4429	CA		Α	309	64.949	66.247	-0.301	1.00	24.93
4431	CB	ILE		309	66.333	66.304	0.411	1.00	24.90
4433		ILE		309	66.333	65.285	1.553		25.34
4436	CD1	ILE		309	67.675	65.077	2.197		27.41
4440	CG2	ILE		309	66.639	67.710	0.943		25.11
4444	С	ILE		309	64.575	67.576	-0.977		25.41
4445	0	ILE		309	64.017	68.468	-0.326		25.21
4446	N	ILE	Α	310	64.848	67.702	-2.274		25.98
4448	CA	ILE	Α	310	64.481	68.928	-3.003		26.46
4450	CB	ILE	Α	310	65.736	69.586	-3.590	1.00	26.50
4452	CG1	ILE		310	66.349	68.722	-4.700	1.00	26.76
4455	CD1	ILE		310	67.350	69.472	-5.530	1.00	27.27
4459	CG2	ILE		310	66.729	69.819	-2.491	1.00	26.11
4463	C	ILE		310	63.393	68.781	-4.066		26.91
4464	0	ILE		310	62.930	69.779	-4.622		26.80
4465	N	GLN		311	62.982	67.543	-4.337		26.94
4467	CA	GLN	Α	311	61.911	67.267	-5.284	1.00	27.25

FIGURE 3 (Cont.) BR

Α	В	С	D	E	F	G	H	I	J
4469	СВ	GLN	Δ	311	62.217	65.999	-6.089	1 00	27.44
4472	CG	GLN		311	63.241	66.219	-7.186		30.05
4475	CD	GLN		311	63.720	64.922	-7.830	1.00	33.37
4476	OE1	GLN		311	64.730	64.920	-8.521	1.00	36.33
4477	NE2	GLN		311	62.999	63.828	-7.606	1.00	34.01
4480	C	GLN		311	60.573	67.102	-4.575	1.00	26.71
4481	0	GLN		311	59.514	67.102	-5.193	1.00	
4482	N	ARG		312	60.620	66.825	-3.280	1.00	
4484	CA	ARG		312	59.418	66.570	-2.503	1.00	
4486	СВ	ARG		312	59.774	66.077	-1.098		25.87
4489	CG	ARG		312	60.382	67.160	-0.225		25.06
4492	CD	ARG		312	61.211	66.630	0.914		23.99
4495	NE	ARG		312	61.963	67.704	1.555		22.64
4497	CZ	ARG		312	61.503	68.481	2.528	1.00	
4498	NH1	ARG		312	62.286	69.429	3.025	1.00	
4501	NH2	ARG		312	60.289	68.325	3.008	1.00	
4504	C	ARG		312	58.558	67.817	-2.386	1.00	
4505	ō	ARG		312	59.053	68.938	-2.448	1.00	
4506	N	ASN		313	57.269	67.601	-2.191	1.00	
4508	CA	ASN		313	56.321	68.702	-2.054	1.00	
4510	CB	ASN		313	55.255	68.594	-3.128	1.00	
4513	CG	ASN		313	55.820	68.829	-4.487	1.00	31.25
4514		ASN		313	56.328	69.921	-4.771	1.00	36.72
4515		ASN		313	55.782	67.807	-5.337		35.16
4518	C	ASN		313	55.711	68.729	-0.676	1.00	
4519	0	ASN		313	54.731	69.426	-0.440	1.00	
4520	N	LYS		314	56.326	67.972	0.234		29.44
4522	CA	LYS		314	55.925	67.944	1.642	1.00	
4524	СВ	LYS		314	54.722	67.029	1.835	1.00	
4527	CG	LYS		314	54.874	65.638	1.202	1.00	
4530	CD	LYS		314	54.635	64.498	2.180	1.00	34.17
4533	CE	LYS		314	53.660	63.459	1.652	1.00	
4536	NZ	LYS	Α	314	54.228	62.656	0.542	1.00	36.19
4540	С	LYS	Α	314	57.081	67.487	2.528	1.00	30.38
4541	0	LYS	Α	314	56.992	67.504	3.759	1.00	30.94
4542	OXT	LYS	Α	314	58.130	67.081	2.028	1.00	30.00
4543	N	ASP	В	17	19.060	6.498	-16.010	1.00	36.37
4545	CA	ASP	В	17	17.827	7.340	-15.968	1.00	36.07
4547	CB	ASP	В	17	16.585	6.454	-15.910	1.00	36.75
4550	CG	ASP	В	17	15.301	7.258	-15.889	1.00	38.21
4551		ASP		17	15.288	8.356	-16.476	1.00	42.09
4552		ASP		17	14.258	6.882	-15.321	1.00	41.73
4553	С	ASP		17	17.853	8.266	-14.742		35.62
4554	0	ASP		17	17.713	7.800	-13.603	1.00	35.09
4557	N	PHE		18	18.002		-14.969		34.42
4559	CA	PHE		18	18.233		-13.845		33.65
4561	CB	PHE		18	18.831		-14.264		33.54
4564	CG	PHE		18	19.286		-13.097		32.06
4565	CD1	PHE		18	20.342	12.202			31.59
4567	CE1	PHE		18	20.747		-11.217		31.53
4569	CZ	PHE		18	20.080		-10.888		30.24
4571	CE2	PHE	В	18	19.029	14.516	-11.638	1.00	31.16

FIGURE 3 (Cont.) BS

A	В	С	D	E	F	G	Н	I	J
4573	CD2	PHE	В	18	18.621	13.779	-12.739	1.00	32.52
4575	С	PHE	В	18	17.015	10.695	-12.946	1.00	33.05
4576	0	PHE	В	18	17.179	10.672	-11.738	1.00	32.55
4577	N		В	19	15.817	10.901	-13.503	1.00	32.85
4578	CA	PRO	В	19	14.606	11.056	-12.680	1.00	32.66
4580	СВ	PRO	В	19	13.497	11.261	-13.722	1.00	32.79
4583	CG	PRO	В	19	14.213	11.795	-14.914	1.00	33.05
4586	CD	PRO	В	19	15.508	11.051	-14.936	1.00	32.96
4589	С	PRO	В	19	14.285	9.869	-11.768	1.00	32.36
4590	0	PRO	В	19	13.759	10.093	-10.685	1.00	31.80
4591	N	GLN	В	20	14.594	8.643	-12.190	1.00	31.98
4593	CA	GLN	В	20	14.399	7.478	-11.329	1.00	32.12
4595	CB	GLN	В	20	14.282	6.175	-12.145	1.00	32.62
4598	CG	GLN	В	20	12.872	5.922	-12.758	1.00	35.79
4601	CD	GLN	В	20	11.784	5.507	-11.736	1.00	38.90
4602	OE1	GLN	В	20	11.382	4.327	-11.677	1.00	40.51
4603	NE2	GLN	В	20	11.292	6.479	-10.956	1.00	40.37
4606	С	GLN		20	15.524	7.368	-10.279	1.00	30.90
4607	0	GLN		20	15.304	6.829	-9.213	1.00	30.46
4608	N	GLN	В	21	16.715	7.872	-10.583	1.00	30.18
4610	CA		В	21	17.778	7.963	-9.575	1.00	30.30
4612	CB	GLN	В	21	19.108	8.421	-10.180	1.00	30.56
4615	CG		В	21	19.929	7.310	-10.799	1.00	33.30
4618	CD		В	21	20.971	6.745	-9.843	1.00	36.37
4619	OE1	GLN		21	21.903	7.457	-9.441	1.00	39.14
4620	NE2	GLN		21	20.822	5.474	-9.479	1.00	36.91
4623	C	GLN		21	17.364	8.924	-8.464	1.00	29.14
4624	0	GLN		21	17.509	8.604	-7.285	1.00	29.47
4625	N	LEU		22	16.838	10.086	-8.841	1.00	27.84
4627	CA	LEU		22	16.384	11.074	-7.864	1.00	27.57
4629	CB	LEU		22	15.793	12.309	-8.546	1.00	27.88
4632	CG		В	22	16.740	13.324	-9.180	1.00	28.18
4634	CD1	LEU		22	15.884	14.370	-9.884	1.00	28.62
4638	CD2	LEU		22	17.667	13.973	-8.145	1.00	28.38
4642	C	LEU		22	15.317	10.478	-6.961	1.00	27.38
4643 4644	0		В	22	15.364	10.643	-5.741	1.00	26.09
	N	GLU GLU		23	14.358 13.207	9.786 9.269	-7.573	1.00	27.02
4646 4648	CA CB	GLU		23 23			-6.847		27.65
4651	CG	GLU		23	12.098 11.022	8.855	-7.825		28.49
4654	CD	GLU		23		7.981	-7.212		32.02
4655	OE1	GLU		23	9.646 9.109	8.256 9.364	-7.782		37.15
4656	OE1	GLU		23	9.109	7.363	-7.545 -8.463		42.58
4657	C	GLU		23	13.618	8.112	-5.938		41.15 26.50
4658	0	GLU		23	13.115	8.008	-4.823		26.62
4659	N	ALA		24	14.513	7.250	-6.421		25.43
4661	CA	ALA		24	15.092	6.179	-5.610		24.85
4663	СВ	ALA		24	16.021	5.297	-6.443		24.98
4667	C	ALA		24	15.864	6.765	-4.421		24.65
4668	Ō	ALA		24	15.827	6.211	-3.318		23.25
4669	N	CYS		25	16.556	7.885	-4.650		24.00
4671	CA	CYS		25	17.315	8.544	-3.589		23.64

FIGURE 3 (Cont.) BT

Α	В	С	D	E	F	G	Н	I	J
4673	СВ	CYS	ъ	25	10 217	9 650	-4.152	1 00	22 72
4676	SG	CYS		25	18.217	9.650			23.72
4677	C				19.117	10.582	-2.885		22.22
		CYS		25	16.374	9.096	-2.524		23.27
4678	0	CYS		25	16.578	8.876	-1.336		23.22
4679	N	VAL		26	15.323	9.779	-2.945		23.25
4681	CA	VAL		26	14.334	10.280	-2.006		23.43
4683	CB	VAL		26	13.175	10.997	-2.725		23.51
4685	CG1	VAL		26	12.005	11.220	-1.804		24.68
4689	CG2	VAL		26	13.650	12.324	-3.276		23.07
4693	С	VAL		26	13.811	9.132	-1.138		23.73
4694	0	VAL		26	13.641	9.300	0.067		23.38
4695	N	LYS	В	27	13.581	7.964	-1.737	1.00	23.54
4697	CA	LYS	В	27	13.012	6.852	-0.972	1.00	24.03
4699	CB	LYS	В	27	12.440	5.765	-1.891	1.00	24.27
4702	CG	LYS	В	27	10.995	6.086	-2.256	1.00	27.21
4705	CD	LYS	В	27	10.544	5.567	-3.606	1.00	31.82
4708	CE	LYS	В	27	9.032	5.811	-3.762	1.00	33.94
4711	NZ	LYS	В	27	8.488	5.279	-5.045	1.00	37.62
4715	С	LYS	В	27	14.026	6.287	-0.004	1.00	22.89
4716	0	LYS	В	27	13.699	6.017	1.145	1.00	23.39
4717	N	GLN	В	28	15.257	6.124	-0.468	1.00	22.27
4719	CA	GLN	В	28	. 16.335	5.645	0.380		21.89
4721	CB	GLN	В	28	17.623	5.496	-0.423		21.61
4724	CG	GLN		28	18.810	4.946	0.352		21.80
4727	CD	GLN		28	18.683	3.471	0.705		23.69
4728	OE1	GLN		28	19.316	2.999	1.657		25.82
4729	NE2	GLN		28	17.882	2.742	-0.054	•	22.57
4732	С	GLN		28	16.518	6.604	1.561		21.61
4733	0	GLN		28	16.596	6.163	2.704		21.00
4734	N	ALA		29	16.556	7.906	1.285		21.58
4736	CA	ALA		29	16.835	8.916	2.323		21.82
4738	СВ	ALA		29	17.120	10.295	1.691		21.91
4742	C	ALA		29	15.684	9.025	3.317		21.73
4743	ō	ALA		29	15.897	9.174	4.508		21.73
4744	N	ASN		30	14.461	8.963	2.822		22.10
4746	CA	ASN		30	13.289	8.996	3.699		22.38
4748	CB	ASN		30	12.013	9.035	2.869		22.05
4751	CG	ASN		30	11.720	10.416	2.319		23.08
4752	OD1			30	12.374	11.387	2.689		22.74
4753	ND2	ASN		30	10.732	10.510	1.424		22.74
4756	C	ASN		30					22.64
4757	0	ASN		30	13.237	7.812	4.655		
4758	N	GLN			12.857	7.962	5.811		22.97
4760	CA	GLN		31	13.604	6.637	4.160		22.84
4762	CB	GLN		31	13.624 13.859	5.438	4.978		23.34
	CG			31		4.210	4.085		23.43
4765		GLN		31	14.118	2.893	4.795		26.33
4768	CD	GLN		31	14.528	1.795	3.815		28.80
4769	OE1	GLN		31	15.700	1.679	3.443		33.07
4770	NE2	GLN		31	13.560	1.007	3.378		32.12
4773	С	GLN		31	14.720	5.582	6.039		23.12
4774	O N	GLN		31	14.542	5.183	7.178		23.43
4775	N	ALA	Ħ	32	15.855	6.146	5.653	1.00	22.32

FIGURE 3 (Cont.)BU

A	В	С	D	E	F	G	Н	I	J
4777	CA	ALA	В	32	16.974	6.318	6.569	1.00	22.90
4779	СВ	ALA		32	18.199	6.814	5.818	1.00	
4783	С	ALA		32	16.590	7.296	7.679	1.00	
4784	0	ALA	В	32	16.750	6.992	8.861	1.00	
4785	N	LEU	В	33	16.069	8.457	7.288	1.00	22.88
4787	CA	LEU		33	15.603	9.462	8.244	1.00	23.19
4789	СВ	LEU		33	14.980	10.661	7.521	1.00	23.23
4792	CG	LEU		33	15.948	11.654	6.869		24.18
4794	CD1	LEU		33	15.253	12.531	5.850	1.00	
4798	CD2	LEU	В	33	16.610	12.528	7.925	1.00	25.95
4802	С	LEU		33	14.565	8.869	9.206	1.00	23.67
4803	0	LEU		33	14.665	9.037	10.415	1.00	
4804	N	SER		34	13.573	8.180	8.654	1.00	
4806	CA	SER		34	12.506	7.580	9.458		25.35
4808	CB	SER		34	11.490	6.887	8.551	1.00	
4811	OG	SER	В	34	10.877	7.830	7.706	1.00	26.80
4813	С	SER		34	13.043	6.579	10.487		25.98
4814	0	SER	В	34	12.547	6.525	11.610		26.04
4815	N	ARG		35	14.062	5.813	10.094		26.60
4817	CA	ARG		35	14.700	4.820	10.962		27.70
4819	CB	ARG		35	15.743	3.993	10.185	1.00	
4822	CG	ARG		35	15.205	2.761	9.484	1.00	
4825	CD	ARG		35	16.207	1.605	9.357	1.00	34.70
4828	NE	ARG	В	35	17.593	2.056	9.140	1.00	
4830	CZ	ARG		35	18.083	2.498	7.984	1.00	
4831	NH1	ARG		35	17.320	2.570	6.914	1.00	34.48
4834	NH2	ARG		35	19.354	2.876	7.903	1.00	33.58
4837	С	ARG		35	15.407	5.464	12.148	1.00	27.46
4838	0	ARG		35	15.465	4.877	13.237	1.00	27.43
4839	N	PHE		36	15.967	6.655	11.926		27.31
4841	CA	PHE	В	36	16.692	7.373	12.965	1.00	26.91
4843	CB	PHE	В	36	17.758	8.289	12.356	1.00	26.72
4846	CG	PHE	В	36	18.835	7.547	11.623	1.00	24.89
4847	CD1	PHE	В	36	19.206	7.916	10.343	1.00	22.57
4849	CE1	PHE	В	36	20.201	7.220	9.656	1.00	
4851	CZ	PHE	В	36	20.845	6.150	10.267	1.00	23.00
4853	CE2	PHE	В	36	20.493	5.777	11.546	1.00	24.18
4855	CD2	PHE	В	36	19.488	6.473	12.224	1.00	24.53
4857	С	PHE	В	36	15.763	8.164	13.851	1.00	27.56
4858	0	PHE	В	36	16.136	8.505	14.964	1.00	28.14
4859	N	ILE	В	37	14.563	8.457	13.357	1.00	28.06
4861	CA	ILE	В	37	13.570	9.208	14.113	1.00	29.01
4863	CB	ILE	В	37	12.677	10.054	13.160	1.00	29.24
4865	CG1	ILE	В	37	13.470	11.240	12.608	1.00	28.43
4868	CD1	ILE		37	12.767	12.003	11.524	1.00	29.06
4872	CG2	ILE		37	11.412	10.552	13.876	1.00	30.14
4876	С	ILE		37	12.719	8.257	14.959	1.00	29.75
4877	0	ILE		37	12.120	8.678	15.948	1.00	30.10
4878	N	ALA		38	12.698	6.977	14.580		30.36
4880	CA	ALA		38	11.784	5.995	15.172	1.00	
4882	CB	ALA		38	11.849	4.666	14.409		30.80
4886	С	ALA	В	38	12.021	5.762	16.651	1.00	30.90

FIGURE 3 (Cont.) BV

A	В	С	D	E	\cdot F	G	Н	I	J
4887	o .	ALA	В	38	11.052	5.739	17.415	1.00	31.31
4888	N	PRO	В	39	13.278	5.595	17.074	1.00	31.28
4889	CA	PRO	В	39	13.573	5.370	18.494	1.00	31.54
4891	СВ	PRO	В	39	15.045	4.922	18.489	1.00	31.77
4894	CG	PRO	В	39	15.425	4.741	17.062	1.00	32.00
4897	CD	PRO	В	39	14.512	5.594	16.270	1.00	31.28
4900	C	PRO	В	39	13.423	6.610	19.377	1.00	31.62
4901	0	PRO	В	39	13.551	6.466	20.594	1.00	32.39
4902	N	LEU	В	40	13.184	7.790	18.794	1.00	30.70
4904	CA	LEU	В	40	13.053	9.012	19.575	1.00	30.07
4906	CB	LEU	В	40	12.980	10.253	18.670	1.00	30.11
4909	CG	LEU		40	14.228	10.593	17.836	1.00	30.37
4911	CD1	LEU	В	40	13.985	11.886	17.056	1.00	30.25
4915	CD2	LEU	В	40	15.502	10.691	18.687	1.00	30.52
4919	С	LEU	В	40	11.801	8.963	20.448	1.00	29.37
4920	0	LEU	В	40	10.747	8.494	20.005	1.00	29.73
4921	N	PRO	В	41	11.903	9.477	21.669	1.00	28.40
4922	CA	PRO	В	41	10.738	9.551	22.553	1.00	28.09
4924	CB	PRO	В	41	11.355	9.872	23.921	1.00	28.24
4927	CG	PRO	В	41	12.658	10.565	23.613	1.00	28.08
4930	CD	PRO	В	41	13.115	10.033	22.301	1.00	28.09
4933	С	PRO	В	41	9.796	10.657	22.100	1.00	27.75
4934	0	PRO	В	41	10.119	11.411	21.154	1.00	26.90
4935	N	PHE	В	42	8.630	10.724	22.739	1.00	27.16
4937	CA	PHE	В	42	7.644	11.774	22.477	1.00	27.19
4939	CB		В	42	8.224	13.158	22.776	1.00	27.06
4942	CG		В	42	8.887	13.259	24.118	1.00	27.64
4943	CD1		В	42	8.136	13.124	25.279	1.00	28.66
4945	CE1	PHE	В	42	8.732	13.207	26.518	1.00	29.45
4947	CZ		В	42	10.096	13.439	26.617	1.00	28.49
4949	CE2		В	42	10.863	13.574	25.475	1.00	27.66
4951	CD2		В	42	10.260	13.485	24.226	1.00	27.57
4953	C		В	42	7.094	11.730	21.053	1.00	27.15
4954	0		В	42	6.729	12.755	20.491	1.00	26.43
4955	N	GLN		43	7.015	10.534	20.489	1.00	27.91
4957	CA CB	GLN		43	6.310	10.320	19.224	1.00	28.60
4959 4962	CG	GLN GLN		43 43	6.294 7.659	8.834 8.201	18.858 18.665	1.00	28.40
4965	CD	GLN		43	8.379	8.718	17.438		28.70 28.74
4966	OE1	GLN		43	7.765	8.927	16.394		29.53
4967	NE2	GLN		43	9.685	8.915	17.558		28.45
4970	C	GLN		43	4.868	10.796	19.363		29.43
4971	ō	GLN		43	4.275	10.720	20.449		30.02
4972	N	ASN		44	4.311	11.291	18.268		30.02
4974	CA	ASN		44	2.942	11.787	18.226		30.82
4976	СВ	ASN		44	1.943	10.631	18.396		31.34
4979	CG	ASN		44	2.264	9.445	17.492		32.36
4980	OD1	ASN		44	2.338	9.579	16.261		35.83
4981	ND2	ASN		44	2.480	8.288	18.096		33.67
4984	C	ASN	В	44	2.684	12.898	19.244	1.00	30.94
4985	0	ASN		44	1.596	12.983	19.805		31.98
4986	N	THR	В	45	3.705	13.716	19.507	1.00	30.13

FIGURE 3 (Cont.) BW

A	В	С	D	E	F	G	H	I	J
4988	CA	THR	R	45	3.529	14.982	20.201	1.00	29.44
4990	CB	THR		45	4.399	15.055	21.470		29.55
4992	OG1	THR		45	5.790	15.106	21.123	1.00	29.59
4994	CG2	THR		45	4.249	13.787	22.313	1.00	30.13
4998	C	THR		45	3.901	16.083	19.216	1.00	28.76
4999	0	THR		45	4.574	15.800	18.231	1.00	29.08
5000	N	PRO		46	3.458	17.318	19.450	1.00	28.09
5001	CA		В	46	3.684	18.421	18.494	1.00	27.28
5003	CB	PRO	В	46	3.174	19.652	19.252	1.00	27.82
5006	CG	PRO	В	46	2.115	19.111	20.181		28.40
5009	CD	PRO	В	46	2.640	17.750	20.605		28.19
5012	C	PRO		46	5.135	18.643	18.041		26.19
5013	0		В	46	5.357	18.854	16.853		25.60
5014	N	VAL	В	47	6.100	18.595	18.957	1.00	24.76
5016	CA	VAL	В	47	7.479	18.902	18.602	1.00	23.94
5018	СВ	VAL	В	47	8.365	19.173	19.859	1.00	24.25
5020	CG1	VAL	В	47	8.593	17.904	20.684	1.00	24.46
5024	CG2	VAL	В	47	9.678	19.801	19.452	1.00	25.37
5028	C	VAL	В	47	8.074	17.824	17.690	1.00	22.86
5029	0	VAL	В	47	8.719	18.150	16.704	1.00	21.98
5030	N	VAL	В	48	7.822	16.549	17.991	1.00	22.17
5032	CA	VAL	В	48	8.303	15.456	17.145	1.00	22.05
5034	CB	VAL	В	48	8.227	14.101	17.872	1.00	22.22
5036	CG1	VAL	В	48	8.620	12.960	16.951	1.00	22.38
5040	CG2	VAL	В	48	9.132	14.128	19.090	1.00	22.62
5044	С	VAL	В	48	7.547	15.414	15.816	1.00	22.15
5045	0	VAL	В	48	8.108	15.076	14.775	1.00	21.53
5046	N	GLU	В	49	6.273	15.760	15.844	1.00	22.30
5048	CA	GLU		49	5.501	15.839	14.612	1.00	23.31
5050	CB	GLU		49	4.020	16.062	14.906	1.00	23.97
5053	CG	GLU		49	3.349	14.847	15.529		27.97
5056	CD	GLU		49	1.902	15.107	15.899	1.00	32.93
5057	OE1	GLU		49	1.410	16.237	15.650	1.00	37.74
5058	OE2	GLU		49	1.263	14.182	16.446	1.00	36.88
5059	С	GLU		49	6.023	16.965	13.727	1.00	22.40
5060	0	GLU		49	6.016	16.837	12.516	1.00	21.26
5061	N	THR		50	6.497	18.044	14.344	1.00	21.39
5063	CA	THR		50	7.105	19.143	13.607		21.78
5065	CB	THR		50	7.382	20.353	14.534		22.24
5067	OG1	THR		50	6.174	20.767	15.191		21.33
5069	CG2	THR		50	7.803	21.573	13.727		22.96
5073	C	THR		50	8.406	18.684	12.964		21.83
5074	0	THR		50	8.671	19.001	11.808		21.23
5075	N	MET		51 51	9.220	17.953	13.728		21.95
5077	CA CB	MET		51 51	10.470	17.408	13.215		21.91
5079 5082	CG	MET MET		51 51	11.207	16.630 17.485	14.299		21.87
5085	SD	MET		51 51	11.735 12.315	16.444	15.441 16.774		20.93
5085	CE	MET		51	13.754	15.689	16.774		22.35
5090	C	MET		51	10.221	16.502	12.014		22.56
5091	0	MET		51	10.221	16.565	11.024		22.83
5092	N	GLN		52	9.179	15.676	12.088		23.09
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FIGURE 3 (Cont.) BX

A	В	C	D	E	F	G	Н	I	J
E004	C D	CT N		50	0 005	14 714	11 016	1 00	00.00
5094	CA	GLN		52 52	8.895	14.714	11.016		23.09
5096	CB	GLN		52 52	7.843	13.694	11.460		23.18
5099	CG	GLN		52 53	8.386	12.700	12.456	1.00	24.11
5102	CD	GLN		52 52	7.334	11.743	12.961	1.00	
5103	OE1	GLN		52	7.463	10.525	12.791	1.00	
5104	NE2	GLN		52	6.304	12.280	13.601	1.00	
5107	C	GLN		52	8.393	15.435	9.787	1.00	
5108	0	GLN		52	8.764	15.123	8.661	1.00	
5109	N	TYR		53	7.531	16.402	10.028	1.00	
5111	CA	TYR		53	6.942	17.213	8.974		22.81
5113	CB	TYR		53	5.939	18.145	9.647		23.23
5116	CG	TYR		53	5.133	19.066	8.784		24.77
5117	CD1	TYR		53	3.855	18.706	8.346	1.00	
5119	CE1	TYR		53	3.089	19.572	7.587	1.00	
5121	CZ	TYR		53	3.582	20.820	7.286	1.00	
5122	OH	TYR		53	2.827	21.673	6.537	1.00	
5124	CE2	TYR		53	4.844	21.209	7.727	1.00	
5126	CD2	TYR		53	5.600	20.335	8.477	1.00	
5128	C	TYR		53	8.051	17.978	8.237	1.00	22.85
5129	0	TYR		53	8.114	17.976	7.010	1.00	
5130	N CA	GLY		54 54	8.948	18.591	9.005	1.00	
5132 5135	CA	GLY GLY		54 54	10.014	19.408 18.608	8.455	1.00	
5136	0	GLY		54 54	11.071		7.738	1.00	22.08
5137	N	ALA		5 4 55	11.669 11.310	19.088 17.384	6.782	1.00	
5139	CA	ALA		55 55	12.382	16.568	8.201 7.656	1.00	
5141	CB	ALA		55 55	12.382	15.714	8.733	1.00	
5145	C	ALA		55 55	11.925	15.714	6.492	1.00	
5146	0	ALA		55	12.692	15.487	5.548	1.00	
5147	N	LEU		56	10.682	15.220	6.538	1.00	
5149	CA	LEU		56	10.265	14.079	5.705		24.30
5151	CB	LEU		56	9.706	12.960	6.586		24.12
5154	CG	LEU		56	10.789	12.220	7.367	1.00	
5156	CD1	LEU		56	10.177	11.362	8.448	1.00	25.81
5160	CD2	LEU		56	11.624	11.386	6.415	1.00	
5164	С	LEU		56	9.241	14.390	4.610	1.00	24.83
5165	0	LEU	В	56	9.168	13.668	3.615		24.82
5166	N	LEU	В	57	8.480	15.459	4.784	1.00	25.44
5168	CA	LEU	В	57	7.363	15.761	3.890		26.38
5170	CB	LEU	В	57	6.196	16.353	4.683	1.00	26.51
5173	CG	LEU	В	57	4.851	15.625	4.607	1.00	29.53
5175	CD1			57	4.953	14.108	4.807	1.00	30.58
5179	CD2	LEU		57	3.880	16.228	5.625	1.00	30.77
5183	С	LEU		57	7.833	16.671	2.741	1.00	
5184	0	LEU		57	7.862	17.895	2.846	1.00	27.01
5185	N	GLY		58	8.237	16.048	1.651		25.60
5187	CA	GLY		58	8.677	16.778	0.477		25.47
5190	C	GLY		58	10.152	17.095	0.529		24.67
5191	0	GLY		58	10.821	16.878	1.542		24.85
5192	N	GLY		59 50	10.655	17.628	-0.575		24.17
5194 5197	CA C	GLY GLY		59 59	12.046	18.001	-0.702		23.50
3171	_	GUI	ם	59	12.688	17.037	-1.671	1.00	23.34

FIGURE 3 (Cont.) BY

Α	В	С	D	E	F	G	Н	I	J
5198	0	GLY	В	59	12.221	15.901	-1.822	1.00	23.79
5199	N	LYS	В	60	13.776	17.465	-2.305		22.25
5201	CA		В	60	14.378	16.698	-3.397	1.00	21.47
5203	СВ	LYS	В	60	14.964	17.634	-4.446	1.00	21.33
5206	CG	LYS	В	60	13.989	18.633	-5.009	1.00	21.64
5209	CD	LYS	В	60	14.690	19.563	-5.983	1.00	20.05
5212	CE	LYS	В	60	15.503	20.635	-5.285	1.00	20.61
5215	NZ	LYS	В	60	14.661	21.571	-4.488	1.00	18.47
5219	C	LYS	В	60	15.473	15.764	-2.916	1.00	20.81
5220	0	LYS	В	60	15.930	14.904	-3.680	1.00	19.71
5221	N	ARG	В	61	15.873	15.934	-1.651	1.00	19.67
5223	CA	ARG	В	61	16.956	15.168	-1.037	1.00	19.66
5225	CB	ARG	В	61	16.531	13.713	-0.785	1.00	19.62
5228	CG	ARG	В	61	15.280	13.581	0.031	1.00	20.32
5231	CD	ARG	В	61	15.456	13.814	1.534	1.00	21.36
5234	NE	ARG	В	61	14.145	13.667	2.159	1.00	22.35
5236	CZ	ARG		61	13.232	14.625	2.243	1.00	24.57
5237	NH1	ARG		61	13.491	15.867	1.836	1.00	25.55
5240	NH2	ARG		61	12.042	14.347	2.754	1.00	25.42
5243	C	ARG		61	18.218	15.188	-1.878	1.00	19.19
5244	0	ARG		61	18.871	14.162	-2.042	1.00	19.59
5245	N	LEU		62	18.575	16.345	-2.419	1.00	18.57
5247	CA	LEU		62	19.781	16.421	-3.233	1.00	18.09
5249	CB	LEU		62	19.801	17.700	-4.043	1.00	18.16
5252	CG	LEU		62	18.659	17.854	-5.069	1.00	17.75
5254	CD1	LEU		62	18.918	19.010	-5.960	1.00	17.68
5258	CD2	LEU		62	18.460	16.582	-5.902	1.00	17.92
5262	С	LEU		62	21.050	16.265	-2.398	1.00	18.27
5263	0	LEU		62	22.075	15.828	-2.904	1.00	19.36
5264	N	ARG		63	20.984	16.589	-1.118	1.00	18.60
5266	CA	ARG		63	22.152	16.472	-0.263	1.00	18.77
5268	CB	ARG		63	22.052	17.389	0.948	1.00	18.34
5271	CG	ARG		63	22.255	18.855	0.557	1.00	18.92
5274	CD	ARG		63 63	21.763	19.861	1.576	1.00	19.63
5277 5279	NE CZ	ARG ARG		63	21.626	21.189	0.993	1.00	18.86
5280	NH1	ARG		63 63		21.574	0.213	1.00	20.23
5283		ARG		63	20.591 19.642	22.816 20.736	-0.258 -0.106	1.00	20.75
5286	C	ARG		63	22.421	14.999			
5287	0	ARG		63	23.547	14.561	0.076 -0.077	1.00	19.10 19.88
5288	N	PRO		64	21.423	14.225	0.504	1.00	19.43
5289	CA	PRO		64	21.423	12.764	0.495	1.00	19.41
5291	CB	PRO		64	20.168	12.704	0.493		20.11
5294	CG	PRO		64	19.619	13.337	1.712	1.00	19.65
5297	CD	PRO		64	20.136	14.628	1.091	1.00	19.55
5300	C	PRO		64	22.061	12.230	-0.851	1.00	18.78
5301	0	PRO		64	22.971	11.411	-0.850	1.00	19.31
5302	N	PHE		65	21.512	12.708	-1.965	1.00	18.78
5304	CA	PHE		65	21.994	12.301	-3.290	1.00	18.13
5306	CB	PHE		65	21.301	13.089	-4.406	1.00	18.17
5309	CG	PHE		65	21.440	12.462	-5.768	1.00	19.67
5310	CD1	PHE	В	65	22.618	12.595	-6.496		21.70

FIGURE 3 (Cont.) BZ

Α	В	С	D	E	F	G	Н	I	J
5312	CE1	PHE	В	65	22.745	12.007	-7.755	1.00	22.62
5314	CZ		В	65	21.697	11.280	-8.296		23.33
5316	CE2	PHE	В	65	20.532	11.138	-7.587	1.00	
5318	CD2	PHE	В	65	20.400	11.730	-6.324	1.00	
5320	C		В	65	23.518	12.444	-3.401	1.00	
5321	ō	PHE	В	65	24.194	11.528	-3.851	1.00	
5322	N	LEU		66	24.042	13.591	-2.986	1.00	
5324	CA	LEU		66	25.470	13.851	-3.011	1.00	
5326	CB	LEU		66	25.775	15.297	-2.615	1.00	
5329	CG	LEU		66	25.431	16.355	-3.650	1.00	
5331	CD1	LEU		66	25.477	17.733	-3.004	1.00	
5335	CD2	LEU		66	26.378	16.312	-4.830	1.00	
5339	C	LEU		66	26.245	12.913	-2.104	1.00	
5340	ō	LEU		66	27.325	12.470	-2.464	1.00	
5341	N	VAL		67	25.717	12.633	-0.920	1.00	
5343	CA	VAL		67	26.388	11.711	-0.011	1.00	
5345	СВ	VAL		67	25.658	11.640	1.340	1.00	
5347	CG1	VAL		67	26.180	10.504	2.196	1.00	
5351	CG2	VAL		67	25.754	13.004	2.088	1.00	
5355	C	VAL		67	26.465	10.322	-0.656	1.00	
5356	0	VAL		67	27.536	9.725	-0.718	1.00	
5357	И	TYR		68	25.315	9.830	-1.120	1.00	
5359	CA	TYR		68	25.226	8.520	-1.767	1.00	
5361	CB	TYR		68	23.790	8.181	-2.162	1.00	
5364	CG	TYR		68	22.884	7.903	-1.001	1.00	
5365	CD1	TYR		68	23.205	6.940	-0.059	1.00	
5367	CE1	TYR		68	22.357	6.678	1.022	1.00	
5369	CZ	TYR		68	21.198	7.396	1.155	1.00	
5370	ОН	TYR		68	20.351	7.135	2.215	1.00	
5372	CE2	TYR		68	20.866	8.363	0.221	1.00	
5374	CD2	TYR		68	21.699	8.599	-0.846	1.00	
5376	C	TYR		68	26.082	8.438	-3.015	1.00	
5377	0	TYR		68	26.788	7.478	-3.201	1.00	
5378	N	ALA		69	26.031	9.456	-3.868	1.00	
5380	CA	ALA		69	26.687	9.377	-5.168	1.00	
5382	CB	ALA		69	26.264	10.525	-6.039	1.00	
5386	С	ALA		69	28.200	9.387	-4.975	1.00	
5387	0	ALA		69	28.960	8.703	-5.696		18.10
5388	N	THR		70	28.639	10.155	-3.985	1.00	
5390	CA	THR		70	30.055	10.258	-3.691	1.00	
5392	CB	THR		70	30.300	11.424	-2.750	1.00	
5394	OG1	THR		70	29.858	12.636	-3.373	1.00	
5396	CG2	THR		70	31.801	11.638	-2.534	1.00	
5400	С	THR		70	30.634	8.968	-3.097	1.00	
5401	0	THR	В	70	31.644	8.449	-3.592	1.00	
5402	N	GLY		71	29.999	8.474	-2.036	1.00	
5404	CA	GLY		71	30.432	7.259	-1.389	1.00	
5407	С	GLY	В	71	30.417	6.071	-2.343	1.00	
5408	0	GLY	В	71	31.314	5.231	-2.310	1.00	
5409	N	HIS	В	72	29.379	6.008	-3.169	1.00	
5411	CA	HIS	В	72	29.201	4.952	-4.163	1.00	21.28
5413	CB	HIS	В	72	27.909	5.167	-4.955	1.00	20.79

FIGURE 3 (Cont.)CA

A	В	C	D	E	F	G	H	I	J
5416	CG	HIS	В	72	26.666	4.749	-4.233	1.00	20.15
5417	ND1		В	72	25.407	4.975	-4.744	1.00	18.98
5419			В	72	24.500	4.502	-3.911	1.00	20.13
5421	NE2		В	72	25.126	3.949	-2.887	1.00	20.13
5423	CD2		В	72	26.482	4.101	-3.059	1.00	21.64
5425	CDZ	HIS		72	30.361	4.878	-5.151	1.00	21.89
5426	0	HIS		72	30.692	3.791	-5.606	1.00	21.76
5427	N	MET		73	30.960	6.023	-5.493	1.00	22.15
5429	CA		В	73 73	32.157	6.023	-6.357	1.00	23.42
5431	CB	MET	В	73	32.672	7.481	-6.565	1.00	23.42
5434	CG	MET	В	73	31.804	8.325	-7.471	1.00	24.99
5437	SD	MET	В	73 73	32.611	9.844	-8.067	1.00	26.07
5438	CE		В	73	33.270	10.463	-6.588		25.93
5442	CE		В	73	33.303	5.200	-5.819		23.68
5443	0		В	73 73	34.094	4.657	-6.595	1.00	
5444	N	PHE	В	74	33.405	5.105	-4.502	1.00	23.69
5446	CA	PHE	В	74	34.474	4.342	-3.856	1.00	23.70
5448	CB	PHE	В	74	35.073	5.171	-2.720	1.00	23.70
5451	CG	PHE		74	35.419	6.571	-3.134	1.00	
5452	CD1	PHE	В	74	34.539	7.620	-2.887	1.00	22.52
5454	CE1	PHE	В	74	34.842	8.909	-3.297	1.00	21.95
5456	CZ	PHE	В	74	36.029	9.160	-3.967	1.00	23.61
5458	CE2		В	74	36.910	8.116	-4.230	1.00	22.42
5460	CD2		В	74	36.604	6.834	-3.818	1.00	23.20
5462	C	PHE	В	74	34.016	2.986	-3.339		23.73
5463	0		В	74	34.751	2.309	-2.625	1.00	23.67
5464	N	GLY		75	32.791	2.607	-3.686	1.00	23.96
5466	CA	GLY		75	32.273	1.287	-3.397	1.00	24.04
5469	C	GLY		75	31.674	1.153	-2.023	1.00	23.99
5470	Ō	GLY		75	31.462	0.038	-1.543	1.00	
5471	N	VAL		76	31.385	2.278	-1.375	1.00	
5473	CA	VAL		76	30.866	2.207	-0.020	1.00	23.08
5475		BVAL		76	31.048	3.547	0.736	0.35	22.92
5476		AVAL		76	31.192	3.459	0.840	0.65	23.42
5479		3VAL		76	30.368	3.508	2.114		22.09
5480	CG1	AVAL	В	76	32.625	3.934	0.590	0.65	23.81
5487	CG21	JAVE	В	76	32.527	3.883	0.872	0.35	23.15
5488	CG2	AVAL	В	76	30.219	4.544	0.625	0.65	24.67
5495	С	VAL	В	76	29.387	1.847	-0.088	1.00	22.55
5496	0	VAL	В	76	28.660	2.300	-0.965		21.42
5497	N	SER	В	77	28.987	0.968	0.819	1.00	22.22
5499	CA	SER	В	77	27.645	0.429	0.868	1.00	22.25
5501	CB	SER	В	77	27.539	-0.621	1.979	1.00	22.22
5504	OG	SER	В	77	26.202	-1.078	2.137	1.00	22.42
5506	C	SER	В	77	26.656	1.550	1.108	1.00	22.33
5507	0	SER	В	77	26.919	2.462	1.898	1.00	21.77
5508	N	THR	В	78	25.534	1.480	0.394	1.00	21.99
5510	CA	THR	В	78	24.431	2.400	0.559		22.06
5512	CB	THR	В	78	23.259	1.990	-0.367		22.16
5514	OG1	THR		78	23.685	2.032	-1.732		23.21
5516	CG2	THR		78	22.126	2.999	-0.303		22.58
5520	C	THR	В	78	23.949	2.433	1.997	1.00	21.59

FIGURE 3 (Cont.)CB

A	В	С	D	E	F	G	Н	I	J
5521	0	THR		78	23.618	3.500	2.527	1.00	21.04
5522	N	ASN		79	23.897	1.261	2.628	1.00	21.29
5524	CA	ASN	В	79	23.467	1.170	4.022	1.00	21.08
5526	CB	ASN	В	79	23.358	-0.293	4.454	1.00	21.68
5529	CG	ASN	В	79	23.046	-0.442	5.923	1.00	21.92
5530	OD1	ASN	В	79	21.903	-0.297	6.343	1.00	23.33
5531	ND2	ASN	В	79	24.060	-0.747	6.706	1.00	22.60
5534	С	ASN	В	79	24.404	1.930	4.963	1.00	20.60
5535	0	ASN	В	79	23.950	2.532	5.920	1.00	19.95
5536	N	THR	В	80	25.708	1.876	4.708	1.00	20.20
5538	CA	THR	В	80	26.661	2.698	5.453	1.00	20.29
5540	CB	THR	В	80	28.086	2.339	5.017	1.00	20.31
5542	OG1	THR	В	80	28.386	1.014	5.482	1.00	20.98
5544	CG2	THR	В	80	29.139	3.242	5.699	1.00	21.55
5548	С	THR	В	80	26.390	4.199	5.257	1.00	20.17
5549	0	THR	В	80	26.440	4.994	6.218	1.00	20.64
5550	N	LEU	В	81	26.078	4.560	4.013	1.00	19.46
5552	CA	LEU	В	81	25.883	5.947	3.604	1.00	19.22
5554	CB	LEU	В	81	25.952	6.044	2.077	1.00	18.97
5557	CG	LEU	В	81	27.376	5.905	1.533	1.00	19.26
5559	CD1	LEU	В	81	27.370	5.638	0.037	1.00	20.15
5563	CD2	LEU		81	28.251	7.121	1.875	1.00	20.46
5567	С	LEU		81	24.584	6.574	4.113	1.00	19.19
5568	0	LEU		81	24.445	7.794	4.139	1.00	18.91
5569	N	ASP		82	23.641	5.746	4.523	1.00	19.51
5571	CA		В	82	22.393	6.219	5.106	1.00	19.28
5573	СВ	ASP	В	82	21.559	5.046	5.616	1.00	19.89
5576	CG		В	82	20.654	4.406	4.552	1.00	21.00
5577	OD1		В	82	20.591	4.823	3.365	1.00	21.03
5578	OD2		В	82	19.938	3.431	4.867	1.00	24.24
5579	С	ASP	В	82	22.645	7.167	6.297	1.00	18.72
5580	0	ASP		82	21.924	8.147	6.462	1.00	18.18
5581	N	ALA		83	23.639	6.861	7.130	1.00	18.70
5583	CA	ALA		83	23.955	7.700	8.290	1.00	19.48
5585	СВ	ALA		83	25.006	7.061	9.204	1.00	19.64
5589	C	ALA		83	24.360	9.113	7.894	1.00	19.16
5590	0	ALA		83	23.679	10.049	8.257	1.00	18.92
5591	N	PRO		84	25.451	9.305	7.163	1.00	19.56
5592	CA	PRO		84	25.781	10.672	6.739	1.00	19.16
5594	СВ	PRO		84	27.114	10.519	6.004	1.00	19.21
5597	CG	PRO		84	27.166	9.070	5.606	1.00	19.67
5600	CD	PRO		84	26.446	8.323	6.694	1.00	19.64
5603	C	PRO		84	24.692	11.299	5.856	1.00	18.58
5604	0	PRO		84	24.509	12.510	5.924	1.00	18.13
5605	N	ALA		85	23.975	10.506	5.063	1.00	18.37
5607	CA	ALA		85	22.891	11.038	4.225	1.00	18.51
5609	СВ	ALA		85	22.314	9.952	3.312	1.00	18.83
5613	С	ALA		85	21.790	11.644	5.073	1.00	18.64
5614	ō	ALA		85	21.313	12.749	4.811	1.00	19.06
5615	N	ALA		86	21.407	10.928	6.114	1.00	18.40
5617	CA	ALA		86	20.360	11.383	7.010	1.00	18.11
5619	CB	ALA		86	19.906	10.245	7.903	1.00	18.05

FIGURE 3 (Cont.)CC

Α	В	С	D	E	F	G	H	I	J
5600	_		_	0.6	00 055	10 566			
5623	C	ALA		86	20.855	12.566	7.841	1.00	17.48
5624	0	ALA		86	20.123	13.505	8.071	1.00	16.95
5625	N	ALA		87	22.105	12.525	8.281	1.00	17.41
5627	CA	ALA		87	22.630	13.600	9.115	1.00	17.40
5629	CB	ALA		87	23.982	13.244	9.638	1.00	17.13
5633	С	ALA		87	22.680	14.917	8.335	1.00	17.61
5634	0	ALA		87	22.298	15.947	8.858	1.00	17.33
5635	N	VAL		88	23.143	14.893	7.091	1.00	18.42
5637	CA	VAL		88	23.208	16.146	6.304	1.00	18.96
5639		BVAL		88	24.038	16.002	4.993	0.35	18.97
5640	CB .	AVAL	В	88	23.983	16.016	4.957	0.65	19.14
5643	CG1	BVAL	В	88	23.256	15.295	3.906	0.35	19.73
5644	CG1	AVAL	В	88	25.429	15.726	5.214	0.65	19.11
5651	CG2	BVAL	В	88	24.517	17.378	4.509	0.35	18.57
5652	CG2	AVAL	В	88	23.381	14.977	4.031	0.65	20.34
5659	С	VAL	В	88	21.813	16.685	6.031	1.00	19.05
5660	0	VAL	В	88	21.610	17.902	6.048	1.00	19.83
5661	N	GLU	В	89	20.858	15.786	5.828	1.00	18.96
5663	CA	GLU	В	89	19.479	16.181	5.611	1.00	19.29
5665	CB	GLU	В	89	18.657	15.024	5.045	1.00	19.83
5668	CG	GLU	В	89	17.271	15.429	4.550	1.00	20.18
5671	CD	GLU	В	89	17.276	16.380	3.353	1.00	21.04
5672	OE1	GLU	В	89	16.175	16.831	2.956	1.00	20.80
5673	OE2	GLU	В	89	18.352	16.669	2.784	1.00	22.55
5674	С	GLU	В	89	18.816	16.727	6.868	1.00	19.09
5675	0	GLU	В	89	17.964	17.587	6.761	1.00	18.76
5676	N	CYS	В	90	19.205	16.246	8.053	1.00	19.19
5678	CA	CYS	В	90	18.694	16.808	9.313	1.00	18.68
5680	CB	CYS	В	90	19.186	16.019	10.519	1.00	19.12
5683	SG	CYS	В	90	18.326	14.474	10.771	1.00	22.59
5684	С	CYS	В	90	19.160	18.255	9.485	1.00	17.90
5685	0	CYS		90	18.407	19.095	9.978	1.00	17.58
5686	N	ILE		91	20.416	18.524	9.129	1.00	16.55
5688	CA	ILE	В	91	20.951	19.877	9.214	1.00	16.20
5690	СВ	ILE		91	22.468	19.934	8.896	1.00	15.98
5692	CG1	ILE	В	91	23.261	19.204	9.970	1.00	15.40
5695	CD1	ILE	В	91	23.203	19.886	11.342	1.00	17.23
5699	CG2	ILE	В	91	22.941	21.391	8.777		15.29
5703	С	ILE		91	20.200	20.722	8.215	1.00	
5704	0	ILE		91	19.770	21.815	8.533	1.00	
5705	N	HIS		92	20.067	20.215	6.992		15.91
5707	CA	HIS		92	19.330	20.914	5.957	1.00	
5709	СВ	HIS		92	19.247	20.072	4.687	1.00	
5712	CG	HIS		92	18.572	20.782	3.567	1.00	
5713		HIS		92	17.518	20.240	2.860	1.00	
5715		HIS		92	17.127	21.104	1.941	1.00	
5717	NE2			92	17.871	22.190	2.043	1.00	19.93
5719		HIS		92	18.776	22.017	3.057	1.00	15.34
5721	C	HIS		92	17.923	21.259	6.424	1.00	
5722	ō	HIS		92	17.524	22.425	6.412	1.00	
5723	N	ALA		93	17.193	20.243	6.885	1.00	
5725	CA	ALA		93	15.809	20.414	7.334	1.00	

FIGURE 3 (Cont.)CD

A	В	С	D	E	F	G	Н	I	J
5727	СВ	ALA	В	93	15.236	19.074	7.793	1.00	17.69
5731	C	ALA		93	15.681	21.456	8.452	1.00	
5732	0	ALA		93	14.806	22.325	8.400	1.00	
5733	N	TYR		94	16.570	21.389	9.449	1.00	
5735	CA	TYR		94	16.550	22.348	10.560	1.00	
5737	СВ	TYR	В	94	17.580	21.968	11.647	1.00	
5740	CG	TYR	В	94	18.635	23.015	11.933	1.00	
5741	CD1	TYR	В	94	18.308	24.219	12.556	1.00	
5743	CE1	TYR	В	94	19.290	25.186	12.809	1.00	
5745	CZ	TYR	В	94	20.601	24.932	12.424	1.00	
5746	OH	TYR	В	94	21.596	25.839	12.653	1.00	22.83
5748	CE2	TYR	В	94	20.935	23.736	11.815	1.00	21.94
5750	CD2	TYR	В	94	19.963	22.802	11.571	1.00	20.83
5752	C	TYR	В	94	16.810	23.765	10.042	1.00	16.90
5753	0	TYR	В	94	16.187	24.727	10.489	1.00	16.75
5754	N	SER	В	95	17.730	23.891	9.098	1.00	16.44
5756	CA	SER	В	95	18.097	25.192	8.581	1.00	17.14
5758	CB	SER	В	95	19.263	25.083	7.593	1.00	16.73
5761	OG	SER	В	95	18.840	24.597	6.337	1.00	18.73
5763	C	SER	В	95	16.887	25.851	7.924	1.00	17.47
5764	0	SER	В	95	16.686	27.050	8.047	1.00	17.44
5765	N	LEU	В	96	16.089	25.064	7.224	1.00	18.06
5767	CA	LEU	В	96	14.897	25.584	6.562	1.00	18.72
5769	CB	LEU	В	96	14.324	24.528	5.642	1.00	19.20
5772	CG	LEU	В	96	15.224	23.982	4.548	1.00	19.55
5774	CD1	LEU	В	96	14.392	23.084	3.642	1.00	21.29
5778	CD2	LEU		96	15.912	25.114	3.771	1.00	19.66
5782	C	LEU		96	13.814	26.018	7.551	1.00	18.78
5783	0	LEU		96	13.179	27.057	7.360	1.00	
5784	N		В	97	13.607	25.227	8.599	1.00	
5786	CA		В	97	12.581	25.536	9.612	1.00	
5788	CB	ILE	В	97	12.525	24.456	10.724	1.00	
5790	CG1	ILE	В	97	12.050	23.122	10.161	1.00	
5793	CD1	ILE	В	97	12.339	21.950	11.075	1.00	
5797	CG2	ILE	В	97	11.617	24.887	11.862	1.00	
5801	C	ILE	В	97	12.874	26.891	10.247	1.00	
5802	0		В	97	11.976	27.698	10.437	1.00	
5803	N	HIS		98	14.142	27.127	10.568		18.85
5805	CA	HIS		98	14.554	28.377	11.204	1.00	
5807	CB	HIS		98	15.891	28.199	11.898	1.00	
5810	CG	HIS		98	15.787	27.494	13.204	1.00	
5811		HIS		98	16.798	27.505	14.135	1.00	
5813 5815		HIS HIS		98 98	16.422	26.803	15.188	1.00	
5817		HIS		98	15.204	26.341 26.756	14.976		19.64
5819	CD2	HIS		98	14.785 14.588	29.526	13.738 10.189	1.00	20.54
5820	0	HIS		98	14.261	30.658	10.189	1.00	
5821	N	ASP		99	14.949	29.218	8.946	1.00	
5823	CA	ASP		99	14.971	30.199	7.861	1.00	
5825	CB	ASP		99	15.515	29.530	6.605	1.00	
5828	CG	ASP		99	15.629	30.470	5.456	1.00	
5829		ASP		99	14.710	30.462	4.590	1.00	

FIGURE 3 (Cont.)CE

Α	В	С	D	E	F	G	Н	I	J
5830	OD2	ASP	В	99	16.618	31.233	5.324	1.00	20.63
5831	C	ASP		99	13.581	30.809	7.572	1.00	18.97
5832	Ō		В	99	13.471	31.985	7.256	1.00	19.10
5833	N	ASP		100	12.537	30.007	7.703	1.00	19.32
5835	CA	ASP	В	100	11.172	30.446	7.448	1.00	20.42
5837	СВ	ASP	В	100	10.283	29.224	7.206	1.00	20.29
5840	CG	ASP	В	100	10.566	28.544	5.883	1.00	20.45
5841	OD1	ASP	В	100	10.363	27.303	5.791	1.00	21.30
5842	OD2	ASP	В	100	10.981	29.158	4.885	1.00	20.64
5843	C	ASP	В	100	10.524	31.287	8.577	1.00	20.97
5844	Ō	ASP	В	100	9.465	31.874	8.372	1.00	21.34
5845	N	LEU		101	11.150	31.332	9.748	1.00	21.55
5847	CA	LEU		101	10.588	31.991	10.925	1.00	22.27
5849	СВ	LEU		101	11.551	31.861	12.120	1.00	22.07
5852	CG	LEU		101	11.746	30.451	12.684	1.00	22.57
5854	CD1	LEU		101	12.901	30.397	13.690	1.00	21.96
5858	CD2	LEU		101	10.471	29.947	13.317	1.00	23.63
5862	C	LEU		101	10.313	33.470	10.646	1.00	22.59
5863	Ō	LEU		101	11.025	34.078	9.870	1.00	22.10
5864	N	PRO		102	9.262	34.035	11.242	1.00	23.34
5865	CA	PRO		102	8.959	35.467	11.096	1.00	23.88
5867	СВ	PRO		102	7.886	35.698	12.152	1.00	23.65
5870	CG	PRO		102	7.151	34.422	12.154	1.00	24.22
5873	CD	PRO		102	8.225	33.347	12.024	1.00	23.27
5876	C	PRO	В	102	10.131	36.428	11.282	1.00	24.08
5877	Ō	PRO		102	10.211	37.387	10.523	1.00	24.64
5878	N	ALA		103	11.019	36.183	12.243	1.00	24.21
5880	CA	ALA		103	12.179	37.054	12.450	1.00	24.56
5882	CB	ALA		103	12.804	36.795	13.823	1.00	24.65
5886	C	ALA		103	13.235	36.885	11.364	1.00	24.37
5887	0	ALA		103	14.092	37.756	11.188	1.00	25.00
5888	N	MET	В	104	13.193	35.747	10.674	1.00	23.93
5890	CA	MET	В	104	14.111	35.445	9.578	1.00	24.35
5892	CB	MET	В	104	14.527	33.969	9.642	1.00	24.14
5895	CG	MET	В	104	15.317	33.629	10.912	1.00	26.61
5898	SD	MET	В	104	17.063	34.058	10.820	1.00	29.08
5899	CE	MET	В	104	17.584	33.058	9.452	1.00	29.15
5903	С	MET	В	104	13.463	35.845	8.237		23.69
5904	0	MET	В	104	13.310	37.040	7.995		23.79
5905	N	ASP	В	105	13.044	34.885	7.404	1.00	23.23
5907	CA	ASP	В	105	12.489	35.198	6.073	1.00	22.98
5909	CB	ASP	В	105	12.936	34.167	5.016	1.00	22.62
5912	CG	ASP	В	105	14.429	34.138	4.838		21.61
5913	OD1	ASP	В	105	14.957	33.260	4.090		18.84
5914	OD2	ASP	В	105	15.163	34.963	5.413	1.00	21.22
5915	С	ASP		105	10.967	35.289	6.067		23.49
5916	0	ASP		105	10.365	35.645	5.054		22.75
5917	N	ASP		106	10.348	34.950	7.185		23.98
5919	CA	ASP		106	8.907	35.099	7.339		25.41
5921	CB	ASP		106	8.567	36.597	7.503		25.60
5924	CG	ASP	В	106	7.203	36.817	8.103	1.00	27.51
5925	OD1	ASP	В	106	6.682	37.941	7.973	1.00	29.77

FIGURE 3 (Cont.)CF

A	В	С	D	E	F	G	H	I	J
			_						
5926		ASP		106	6.583	35.930	8.728	1.00	
5927	C	ASP		106	8.126	34.503	6.172	1.00	
5928	0	ASP		106	7.385	35.206	5.498	1.00	
5929	N	ASP		107	8.309	33.203	5.936	1.00	
5931	CA	ASP	В	107	7.630	32.487	4.861	1.00	
5933	CB	ASP	В	107	8.641	31.685	4.032	1.00	
5936	CG	ASP	В	107	9.212	32.477	2.895	1.00	
5937			В	107	8.428	32.869	2.004	1.00	
5938		ASP		107	10.426	32.755	2.786	1.00	
5939	C	ASP		107	6.573	31.549	5.403		26.02
5940	0	ASP		107	6.773	30.883	6.425		26.50
5941	N CA	ASP		108	5.443	31.487	4.703	1.00	
5943 5945	CA CB	ASP		108	4.331	30.628	5.107	1.00	
5945	CG	ASP		108	3.012	31.404	5.131	1.00	
5949		ASP ASP		108	2.611	31.970	3.766	1.00	
5950	OD1	ASP		108 108	1.460	32.426	3.651	1.00	
5951	C C	ASP			3.356	32.024	2.762	1.00	
5951	0	ASP		108 108	4.183 3.362	29.359	4.260	1.00	24.50 23.73
5952	N	LEU		109	4.975	28.516 29.228	4.588 3.197		23.73
5955	CA	LEU		109	4.939	28.054	2.323		23.97
5957	CB	LEU		109	4.386	28.414	0.940		24.10
5960	CG	LEU		109	2.907	28.201	0.569	1.00	
5962	CD1	LEU		109	2.748	28.570	-0.917	1.00	
5966	CD2	LEU		109	2.748	26.794	0.840	1.00	
5970	C	LEU		109	6.329	27.462	2.103	1.00	
5971	0	LEU		109	7.271	28.178	1.813	1.00	
5972	N	ARG		110	6.426	26.146	2.208	1.00	
5974	CA	ARG		110	7.609	25.422	1.776	1.00	
5976	CB	ARG		110	8.662	25.359	2.878		22.08
5979	CG	ARG		110	9.916	24.624	2.441		21.74
5982	CD	ARG		110	11.021	24.622	3.487	-	19.15
5985	NE	ARG		110	11.586	25.949	3.737	1.00	
5987	CZ	ARG		110	12.421	26.579	2.911	1.00	
5988		ARG		110	12.900	27.771	3.239	1.00	
5991	NH2	ARG		110	12.789	26.027	1.770	1.00	
5994	С	ARG		110	7.210	24.022	1.382	1.00	
5995	0	ARG	В	110	6.409	23.385	2.071	1.00	
5996	N	ARG		111	7.789	23.549	0.283		22.18
5998	CA	ARG		111	7.542	22.212	-0.244		22.54
6000	CB	ARG	В	111	8.143	21.147	0.679		22.32
6003	CG	ARG	В	111	9.662	21.147	0.734		21.77
6006	CD	ARG	В	111	10.202	20.545	2.021		21.80
6009	NE	ARG	В	111	11.633	20.275	1.973		20.78
6011	CZ	ARG	В	111	12.305	19.671	2.947	1.00	20.45
6012	NH1	ARG	В	111	11.688	19.269	4.048	1.00	18.82
6015	NH2	ARG		111	13.608	19.464	2.826	1.00	19.98
6018	С	ARG		111	6.042	21.973	-0.465		23.08
6019	0	ARG		111	5.544	20.861	-0.338		22.39
6020	N	GLY		112	5.335	23.042	-0.807		23.92
6022	CA	GLY		112	3.921	22.975	-1.135		24.69
6025	С	GLY	В	112	3.010	23.023	0.070	1.00	24.98

FIGURE 3 (Cont.)CG

Α	В	С	D	E	F	G	Н	I	J
6026	0	GLY	В	112	1.808	22.978	-0.089	1.00	25.54
6027	N	LEU	В	113	3.578	23.126	1.268	1.00	25.57
6029	CA		В	113	2.813	23.045	2.508	1.00	25.94
6031	CB	LEU	В	113	3.226	21.797	3,283	1.00	26.65
6034	CG	LEU	В	113	3.068	20.468	2.548	1.00	29.36
6036	CD1	LEU		113	3.750	19.369	3.338	1.00	31.10
6040	CD2	LEU	В	113	1.599	20.127	2.336	1.00	31.06
6044	С	LEU	В	113	3.043	24.272	3.388	1.00	25.32
6045	0	LEU	В	113	4.027	24.999	3.216	1.00	24.34
6046	N	PRO	В	114	2.153	24.497	4.355	1.00	25.34
6047	CA		В	114	2.425	25.500	5.383	1.00	24.92
6049	СВ	PRO	В	114	1.261	25.331	6.348	1.00	25.42
6052	CG	PRO		114	0.165	24.734	5.503	1.00	25.33
6055	CD	PRO		114	0.862	23.812	4.575	1.00	25.09
6058	С	PRO	В	114	3.764	25.201	6.077	1.00	24.65
6059	0	PRO	В	114	4.051	24.057	6.403	1.00	24.29
6060	N	THR	В	115	4.583	26.222	6.259	1.00	24.42
6062	CA	THR	В	115	5.850	26.062	6.966	1.00	24.49
6064	CB	THR	В	115	6.635	27.364	6.990	1.00	24.32
6066	OG1	THR	В	115	5.798	28.437	7.465	1.00	26.32
6068	CG2	THR	В	115	7.058	27.773	5.573	1.00	24.50
6072	С	THR	В	115	5.607	25.577	8.387	1.00	24.50
6073	0	THR	В	115	4.512	25.721	8.944	1.00	23.20
6074	N	CYS	В	116	6.641	24.995	8.969	1.00	24.26
6076	CA	CYS	В	116	6.537	24.419	10.297	1.00	24.93
6078	CB	CYS	В	116	7.885	23.869	10.759	1.00	24.70
6081	SG	CYS	В	116	8.346	22.384	9.881	1.00	26.74
6082	C	CYS	В	116	6.002	25.412	11.305	1.00	24.67
6083	0		В	116	5.204	25.042	12.148	1.00	25.48
6084	N		В	117	6.408	26.672	11.212	1.00	24.78
6086	CA		В	117	5.981	27.647	12.214	1.00	25.04
6088	CB		В	117	6.888	28.867	12.233	1.00	25.27
6091	CG	HIS		117	6.649	29.828	11.116	1.00	25.24
6092			В	117	5.983	31.018	11.293	1.00	26.70
6094	CE1		В	117	5.924	31.663	10.141	1.00	27.42
6096	NE2	HIS	В	117	6.532	30.935	9.226	1.00	26.41
6098		HIS		117	6.985	29.776	9.807	1.00	26.27
6100	C	HIS		117	4.539	28.076	12.018		25.01
6101	0	HIS		117	3.891	28.466	12.971		25.49
6102	N	VAL		118	4.051	28.021	10.784		25.12
6104	CA	VAL		118	2.631	28.253	10.508		25.25
6106 6108	CB CC1	VAL VAL		118	2.394	28.567	9.018		25.46
6112	CG2	VAL		118 118	0.884 3.035	28.609 29.894	8.673		26.21
6116	C	VAL		118	1.786		8.681 10.999		25.70
6117	0	VAL		118	0.821	27.078 27.285	11.720		25.08 24.86
6118	N	LYS		119	2.167	25.856	10.639		25.25
6120	CA	LYS		119	1.439	24.654	11.042		25.25
6122	СВ	LYS		119	1.935	23.428	10.263		26.25
6125	CG	LYS		119	0.884	22.726	9.418		28.80
6128	CD	LYS		119	-0.165	22.025	10.250		31.95
6131	CE	LYS		119	-0.978	21.015	9.432		33.31

FIGURE 3 (Cont.)CH

Α	В	C	D	E	F	G	H	I	J
6134	NZ	LYS		119	-1.864	21.671	8.417		34.97
6138	С	LYS		119	1.468	24.365	12.564		25.31
6139	0	LYS		119	0.445	24.061	13.161		24.99
6140	N	PHE	В	120	2.626	24.488	13.193		24.69
6142	CA	PHE	В	120	2.789	24.032	14.567		24.30
6144	CB		В	120	3.908	22.993	14.616		24.16
6147	CG	PHE		120	3.639	21.763	13.799		24.65
6148	CD1	PHE		120	2.915	20.704	14.332		26.16
6150	CE1	PHE		120	2.690	19.541	13.582	1.00	25.66
6152	CZ	PHE		120	3.192	19.441	12.311	1.00	25.37
6154	CE2	PHE		120	3.930	20.494	11.767	1.00	24.54
6156	CD2	PHE	В	120	4.158	21.637	12.513	1.00	25.35
6158	С	PHE	В	120	3.084	25.165	15.565	1.00	23.77
6159	0	PHE	В	120	3.155	24.927	16.752	1.00	23.66
6160	N	GLY	В	121	3.250	26.391	15.083	1.00	23.69
6162	CA	GLY	В	121	3.622	27.516	15.935	1.00	23.51
6165	C	GLY	В	121	5.130	27.773	15.955	1.00	23.55
6166	0	GLY	В	121	5.927	26.892	15.652	1.00	22.34
6167	N	GLU	В	122	5.518	28.986	16.320	1.00	23.70
6169	CA	GLU	В	122	6.934	29.381	16.314	1.00	24.67
6171	CB	GLU	В	122	7.091	30.868	16.639	1.00	24.89
6174	CG	GLU	В	122	6.990	31.777	15.427	1.00	27.84
6177	CD	GLU	В	122	7.069	33.248	15.796		30.34
6178	OE1	GLU	В	122	8.174	33.721	16.136		35.10
6179	OE2	GLU	В	122	6.033	33.931	15.743		32.39
6180	С	GLU	В	122	7.792	28.558	17.283		24.12
6181	0	GLU	В	122	8.925	28.199	16.955		23.74
6182	N	ALA	В	123	7.249	28.292	18.469		23.52
6184	CA	ALA	В	123	7.968	27.587	19.526		23.88
6186	CB	ALA	В	123	7.156	27.594	20.816		23.93
6190	С	ALA	В	123	8.287	26.159	19.098		23.98
6191	0	ALA	В	123	9.417	25.688	19.247		22.97
6192	N	ASN		124	7.290	25.494	18.524		23.86
6194	CA	ASN		124	7.484	24.159	17.980		24.09
6196	CB	ASN	В	124	6.165	23.561	17.486		24.26
6199	CG	ASN	В	124	5.365	22.896	18.601	1.00	
6200	OD1	ASN	В	124	4.125	22.946	18.602	1.00	
6201	ND2	ASN	В	124	6.064	22.278	19.561	1.00	23.40
6204	С	ASN		124	8.508	24.168	16.849		23.11
6205	0	ASN		124	9.294	23.250	16.750		22.29
6206	N	ALA		125	8.496	25.208	16.015		22.58
6208	CA	ALA		125	9.430	25.303	14.896		22.31
6210	СВ	ALA		125	9.043	26.425	13.953		23.02
6214	С	ALA		125	10.836	25.526	15.405		21.81
6215	0	ALA		125	11.766	24.906	14.932	1.00	
6216	N	ILE		126	10.985	26.419	16.371	1.00	
6218	CA	ILE		126	12.293	26.701	16.936		20.84
6220	СВ	ILE		126	12.177	27.795	18.007		20.71
6222	CG1	ILE		126	11.994	29.168	17.339		21.50
6225	CD1	ILE		126	11.342	30.199	18.243		22.29
6229	CG2	ILE		126	13.395	27.816	18.903		21.11
6233	С	ILE	В	126	12.888	25.423	17.523		19.99

FIGURE 3 (Cont.)CI

6234 O ILE B 126	Α	В	C	D	E	F	G	Н	I	J
6235 N LEU B 127 12.522 23.553 19.061 1.00 19.20 6239 CB LEU B 127 11.477 23.141 20.106 1.00 19.23 6242 CG LEU B 127 11.477 24.029 21.357 1.00 20.75 6244 CD1 LEU B 127 10.382 23.528 22.321 1.00 22.65 6252 C LEU B 127 10.382 23.528 22.321 1.00 12.66 6253 O LEU B 127 13.757 21.682 18.244 1.00 18.61 6254 N ALA B 128 11.926 22.286 17.082 1.00 18.61 6255 C ALA B 128 12.073 21.218 16.108 1.00 19.13 6254 N ALB B 128 13.373 21.368 15.315 1.00 18.59 6264 N	6234	0	TLE	R	126	14.037	25.072	17 234	1 00	19 91
6237 CA LEU B 127 11.477 23.141 20.106 1.00 19.20 6242 CG LEU B 127 11.417 24.029 21.357 1.00 20.75 6244 CD1 LEU B 127 12.776 24.131 22.047 1.00 22.13 6252 C LEU B 127 10.382 23.528 22.321 1.00 19.26 6253 O LEU B 127 13.757 21.682 18.244 1.00 19.51 6254 N ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 11.926 22.286 17.082 1.00 18.61 6265 CA ALA B 128 12.073 21.183 15.181 1.00 18.51 6262 C ALA B 128 14.079 20.387 15.065 1.00 18.59 6262 C										
6239 CB LEU B 127 11.477 23.141 20.106 1.00 19.23 6244 CDI LEU B 127 11.417 24.029 21.357 1.00 22.13 6248 CD2 LEU B 127 10.382 23.528 22.321 1.00 22.65 6252 C LEU B 127 12.776 22.413 18.096 1.00 19.26 6253 O LEU B 127 13.757 21.662 18.244 1.00 19.26 6256 CA ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 10.873 21.183 15.181 1.00 18.59 6262 C ALA B 128 10.873 21.368 15.315 1.00 18.59 6262 C ALA B 128 14.079 20.387 15.065 1.00 18.59 6264 N GLY B 129 14.948 22.879 14.272 1.00 18.59 <td></td>										
6242 CG CEU B 127 11,417 24,029 21,357 1.00 20,75 6248 CD2 LEU B 127 10,382 23,528 22,321 1.00 22,65 6252 C LEU B 127 10,382 23,528 22,321 1.00 19,26 6253 O LEU B 127 13,757 21,682 18,244 1.00 19,26 6254 N ALA B 128 11,926 22,286 17,082 1.00 18,61 6256 CA ALA B 128 12,073 21,218 16,108 1.00 19,13 6258 CB ALA B 128 10,873 21,183 15,181 1.00 18,61 6262 C ALA B 128 14,079 20,387 15,065 1.00 18,99 6264 N GLY B 129 13,685 22,595 14,916 1.00 18,99 6265 CA GLY B 129 16,177 22,879 14,272 1.00 18,99 6267 O GLY B 129 16,946 22,879 14,272 1.00 18,99 <td></td>										
6244 CD1 LEU B 127 12.776 24.131 22.047 1.00 22.13 6248 CD2 LEU B 127 10.382 23.528 22.321 1.00 19.26 6253 O LEU B 127 13.757 21.682 18.244 1.00 19.51 6254 N ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 10.873 21.183 15.181 1.00 18.61 6262 C ALA B 128 10.873 21.183 15.315 1.00 18.64 6263 O ALA B 128 14.079 20.387 15.065 1.00 18.59 6264 N GLY B 129 14.948 22.879 14.727 1.00 18.99 6270 O GLY B 129 16.117 22.574 15.200 1.00 18.99 6271 N										
6248 CD2 LEU B 127 10.382 23.528 22.321 1.00 22.65 6252 C LEU B 127 12.776 22.413 18.096 1.00 19.26 6254 N ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 12.073 21.218 16.108 1.00 18.61 6258 CB ALA B 128 10.873 21.318 15.181 1.00 18.64 6262 C ALA B 128 14.079 20.387 15.065 1.00 18.99 6264 N GLY B 129 13.685 22.595 14.916 1.00 18.99 6266 CA GLY B 129 14.179 22.574 15.200 1.00 18.99 6267 O GLY B 129 17.098 21.959 14.790 1.00 18.66 6273 CA										
6252 C LEU B 127 12.776 22.413 18.096 1.00 19.26 6253 N ALA B 128 11.926 22.286 17.082 1.00 19.51 6256 CA ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 12.073 21.218 16.108 1.00 19.13 6252 C ALA B 128 10.873 21.183 15.085 1.00 18.57 6263 O ALA B 128 14.079 20.387 15.065 1.00 18.99 6264 N GLY B 129 13.685 22.595 14.916 1.00 18.59 6266 CA GLY B 129 13.085 22.595 14.916 1.00 18.59 6269 C GLY B 129 16.17 22.574 15.200 1.00 18.59 6279 O GLY B 129 17.098 21.959 14.797 1.00 18.49										
6253 O LEU B 127 13.757 21.682 18.244 1.00 19.51 6256 CA ALA B 128 11.926 22.286 17.082 1.00 18.61 6258 CA ALA B 128 12.073 21.218 16.108 1.00 18.64 6258 CB ALA B 128 13.373 21.368 15.315 1.00 18.59 6264 N GLY B 129 13.685 22.595 14.916 1.00 18.59 6266 CA GLY B 129 14.948 22.879 14.272 1.00 18.59 6270 O GLY B 129 17.098 21.959 14.790 1.00 18.59 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.11 6275 CB ASP B 130 17.061 22.771 17.457 1.00 19.02 6275 CB										
6254 N ALA B 128 11.926 22.286 17.082 1.00 18.61 6256 CA ALA B 128 12.073 21.218 16.108 1.00 18.64 6258 CB ALA B 128 10.873 21.183 15.181 1.00 18.64 6262 C ALA B 128 13.373 21.368 15.315 1.00 18.99 6264 N GLY B 129 13.685 22.579 14.916 1.00 18.99 6269 C GLY B 129 14.948 22.879 14.272 1.00 18.99 6270 O GLY B 129 17.098 21.959 14.790 1.00 18.99 6273 CA ASP B 130 16.017 22.574 15.200 1.00 18.66 6271 N ASP B 130 16.017 22.571 17.457 1.00 18.66 6273 CA ASP B 130 17.061 22.771 17.457 1.00 18.49										
6256 CA ALA B 128		N	ALA	В		11.926				
6262 C ALA B 128 13.373 21.368 15.315 1.00 18.57 6263 O ALA B 128 14.079 20.387 15.065 1.00 18.99 6264 N GLY B 129 13.685 22.595 14.916 1.00 18.59 6269 C GLY B 129 16.117 22.574 15.200 1.00 18.59 6270 O GLY B 129 16.117 22.574 15.200 1.00 18.69 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.02 6273 CA ASP B 130 16.652 23.327 18.829 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 18.48 6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.14 6281 C ASP B 130 16.221 25.488 19.889 1.00 18.36	6256	CA	ALA	В	128	12.073	21.218			
6263 O ALA B 128 14.079 20.387 15.065 1.00 18.99 6264 N GLY B 129 13.685 22.595 14.916 1.00 18.59 6269 C GLY B 129 16.117 22.574 15.200 1.00 18.99 6270 O GLY B 129 17.098 21.959 14.790 1.00 18.66 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.02 6273 CA ASP B 130 16.652 23.327 18.829 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 19.12 6278 CB ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 16.629 17.878 1.00 19.13 6281 C ASP B 130 16.221 25.488 19.899 1.00 20.44 62	6258	CB	ALA	В	128	10.873	21.183		1.00	18.64
6264 N GLY B 129 13.685 22.595 14.916 1.00 18.99 6266 CA GLY B 129 14.948 22.879 14.272 1.00 18.59 6270 O GLY B 129 17.098 21.959 14.790 1.00 18.99 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.11 6273 CA ASP B 130 16.652 23.327 18.829 1.00 19.11 6275 CB ASP B 130 16.652 23.327 18.829 1.00 18.48 6278 CG ASP B 130 16.652 23.327 18.881 1.00 19.13 6280 OD2 ASP B 130 17.086 25.482 17.880 1.00 19.13 6281 C ASP B 130 18.481	6262	C	ALA	В	128	13.373	21.368	15.315	1.00	18.57
6266 CA GLY B 129 14.948 22.879 14.272 1.00 18.59 6269 C GLY B 129 16.117 22.574 15.200 1.00 18.99 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.01 6273 CA ASP B 130 16.652 23.327 18.829 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 19.02 6279 OD1 ASP B 130 16.654 24.851 18.881 1.00 20.10 6280 OD2 ASP B 130 17.344 21.283 17.586 1.00 18.48 6281 C ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 16.213 <td>6263</td> <td>0</td> <td>ALA</td> <td>В</td> <td>128</td> <td>14.079</td> <td>20.387</td> <td>15.065</td> <td>1.00</td> <td>18.99</td>	6263	0	ALA	В	128	14.079	20.387	15.065	1.00	18.99
6269 C GLY B 129 16.117 22.574 15.200 1.00 18.99 6270 O GLY B 129 17.098 21.959 14.790 1.00 18.66 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.01 6273 CA ASP B 130 16.652 23.327 18.829 1.00 19.02 6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 16.654 24.851 18.881 1.00 19.13 6280 OD2 ASP B 130 17.344 21.283 17.586 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.36 6281 CA ALA B 131 16.274 <td>6264</td> <td>N</td> <td>GLY</td> <td>В</td> <td>129</td> <td>13.685</td> <td>22.595</td> <td>14.916</td> <td>1.00</td> <td>18.91</td>	6264	N	GLY	В	129	13.685	22.595	14.916	1.00	18.91
6270 O GLY B 129 17.098 21.959 14.790 1.00 18.66 6271 N ASP B 130 16.001 22.986 16.459 1.00 19.11 6273 CA ASP B 130 17.061 22.771 17.457 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 18.48 6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 18.481 20.860 17.575 1.00 18.36 6283 N ALA B 131 16.274 20.506 17.675 1.00 18.43 6285 CA ALA B 131 16.347 19.069 17.878 1.00 18.43 6285 CA ALA B 131 17.407 17.248	6266	CA	GLY	В	129	14.948	22.879	14.272	1.00	18.59
6271 N ASP B 130 16.001 22.986 16.459 1.00 19.11 6273 CA ASP B 130 17.061 22.771 17.457 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 19.02 6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 17.344 21.283 17.586 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.48 6285 CA ALA B 131 16.274 20.506 17.675 1.00 18.43 6287 CB ALA B 131 16.347 19.069 17.878 1.00 18.43 6287 CB </td <td>6269</td> <td>С</td> <td>GLY</td> <td>В</td> <td>129</td> <td>16.117</td> <td>22.574</td> <td>15.200</td> <td>1.00</td> <td>18.99</td>	6269	С	GLY	В	129	16.117	22.574	15.200	1.00	18.99
6273 CA ASP B 130 17.061 22.771 17.457 1.00 19.02 6275 CB ASP B 130 16.652 23.327 18.829 1.00 18.48 6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 17.344 21.283 17.586 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.36 6283 N ALA B 131 16.247 20.506 17.675 1.00 18.43 6285 CA ALA B 131 15.012 <td>6270</td> <td>0</td> <td>GLY</td> <td>В</td> <td>129</td> <td>17.098</td> <td>21.959</td> <td>14.790</td> <td>1.00</td> <td>18.66</td>	6270	0	GLY	В	129	17.098	21.959	14.790	1.00	18.66
6275 CB ASP B 130 16.652 23.327 18.829 1.00 18.48 6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 18.481 20.860 17.541 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.36 6283 N ALA B 131 16.274 20.506 17.675 1.00 18.43 6285 CA ALA B 131 15.012 18.540 18.344 1.00 18.33 6287 CB ALA B 131 17.407 <td>6271</td> <td>N</td> <td>ASP</td> <td>В</td> <td>130</td> <td>16.001</td> <td>22.986</td> <td>16.459</td> <td>1.00</td> <td>19.11</td>	6271	N	ASP	В	130	16.001	22.986	16.459	1.00	19.11
6278 CG ASP B 130 16.654 24.851 18.881 1.00 20.10 6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 18.481 20.860 17.541 1.00 18.36 6283 N ALA B 131 16.274 20.506 17.675 1.00 18.43 6285 CA ALA B 131 16.347 19.069 17.878 1.00 18.43 6287 CB ALA B 131 15.012 18.540 18.344 1.00 18.51 6287 CB ALA B 131 17.407 17.248 16.748 1.00 18.45 6291 N LEU B 132 16.518 <td>6273</td> <td>CA</td> <td>ASP</td> <td>В</td> <td>130</td> <td>17.061</td> <td>22.771</td> <td>17.457</td> <td>1.00</td> <td>19.02</td>	6273	CA	ASP	В	130	17.061	22.771	17.457	1.00	19.02
6279 OD1 ASP B 130 17.086 25.482 17.880 1.00 19.13 6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 17.344 21.283 17.586 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.36 6283 N ALA B 131 16.274 20.506 17.675 1.00 18.43 6285 CA ALA B 131 16.347 19.069 17.878 1.00 18.51 6287 CB ALA B 131 15.012 18.540 18.344 1.00 18.33 6291 C ALA B 131 17.407 17.248 16.629 1.00 18.44 6292 O ALA B 132 16.518 18.850 15.445 1.00 18.17 6295 CA LEU B 132						16.652		18.829	1.00	18.48
6280 OD2 ASP B 130 16.221 25.488 19.889 1.00 20.44 6281 C ASP B 130 17.344 21.283 17.586 1.00 18.66 6282 O ASP B 130 18.481 20.860 17.541 1.00 18.36 6283 N ALA B 131 16.274 20.506 17.675 1.00 18.43 6285 CA ALA B 131 16.347 19.069 17.878 1.00 18.51 6287 CB ALA B 131 15.012 18.540 18.344 1.00 18.33 6291 C ALA B 131 17.407 17.248 16.629 1.00 18.44 6292 O ALA B 132 16.518 18.850 15.445 1.00 18.67 6293 N LEU B 132 16.518 18.850 15.445 1.00 18.17 6295 CA										
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	6331	CA	THR	В	134	21.121	17.657	17.476	1.00	18.15
6335 OG1 THR B 134 20.296 19.101 19.283 1.00 18.94										
	6335	OG1	THR	В	134	20.296	19.101	19.283	1.00	18.94

FIGURE 3 (Cont.)CJ

A	В	С	D	E	F	G	Н	I	J
6337	CG2	THR	В	134	21.169	17.017	19.864	1.00	19.06
6341	C	THR		134	21.060	16.225	16.950	1.00	18.22
6342	0	THR		134	22.014	15.474	17.106	1.00	18.09
6343	N	LEU		135	19.936	15.870	16.322	1.00	17.83
6345	CA	LEU		135	19.739	14.530	15.781	1.00	17.43
6347	СВ	LEU		135	18.336	14.416	15.184	1.00	17.61
6350	CG	LEU		135	18.006	13.113	14.455	1.00	18.78
6352	CD1	LEU		135	18.167	11.908	15.367	1.00	18.23
6356	CD2	LEU		135	16.619	13.201	13.912	1.00	19.31
6360	С	LEU	В	135	20.818	14.186	14.743	1.00	16.77
6361	0	LEU		135	21.287	13.045	14.664	1.00	16.01
6362	N	ALA		136	21.243	15.179	13.970	1.00	16.82
6364	CA	ALA		136	22.280	14.960	12.974	1.00	16.89
6366	CB	ALA		136	22.581	16.241	12.231	1.00	17.47
6370	С	ALA		136	23.548	14.406	13.625	1.00	17.27
6371	0	ALA	В	136	24.184	13.484	13.091	1.00	17.46
6372	N	PHE	В	137	23.888	14.943	14.789	1.00	17.08
6374	CA	PHE	В	137	25.088	14.528	15.496	1.00	17.65
6376	CB	PHE	В	137	25.593	15.666	16.381	1.00	18.03
6379	CG	PHE	В	137	26.007	16.88Ò	15.584	1.00	18.67
6380	CD1	PHE	В	137	25.230	18.019	15.566	1.00	18.86
6382	CE1	PHE	В	137	25.605	19.122	14.809	1.00	19.97
6384	CZ	PHE	В	137	26.757	19.070	14.029	1.00	19.23
6386	CE2		В	137	27.526	17.940	14.023	1.00	19.82
6388	CD2	PHE	В	137	27.140	16.835	14.788	1.00	21.06
6390	С	PHE	В	137	24.848	13.218	16.260	1.00	17.89
6391	0	PHE	В	137	25.764	12.440	16.419	1.00	17.92
6392	N	SER	В	138	23.613	12.966	16.699	1.00	18.09
6394	CA	SER	В	138	23.275	11.661	17.269	1.00	18.71
6396	CB	SER	В	138	21.839	11.634	17.769	1.00	18.28
6399	OG	SER	В	138	21.712	12.386	18.950	1.00	19.32
6401	С	SER	В	138	23.466	10.571	16.212	1.00	18.94
6402	0	SER	В	138	24.084	9.555	16.485	1.00	19.25
6403	N	ILE		139	22.967	10.819	15.001	1.00	19.22
6405	CA	ILE		139	23.123	9.884	13.890	1.00	19.25
6407	CB	ILE		139	22.430	10.403	12.622	1.00	19.39
6409	CG1	ILE		139	20.916	10.363	12.822	1.00	18.95
6412	CD1	ILE		139	20.144	11.100	11.805		21.43
6416	CG2	ILE		139	22.848	9.571	11.387		17.88
6420	С	ILE		139	24.606	9.609	13.612		19.87
6421	0	ILE		139	25.021	8.461	13.593		19.68
6422	N	LEU		140	25.397	10.648	13.393		19.88
6424	CA	LEU		140	26.799	10.451	13.025		20.40
6426	CB	LEU		140	27.452	11.764	12.620		20.25
6429	CG	LEU		140	27.071	12.298	11.246		20.51
6431		LEU		140	27.798	13.593	11.005		23.24
6435	CD2			140	27.402	11.299	10.149		21.98
6439	С	LEU		140	27.600	9.803	14.145		20.89
6440	0	LEU		140	28.572	9.088	13.876		21.00
6441	N	SER		141	27.211	10.045	15.396		21.26
6443	CA	SER		141	27.933	9.439	16.514		22.16
6445	СВ	SER	В	141	27.926	10.329	17.756	1.00	21.93

FIGURE 3 (Cont.)CK

Α	В	С	D	E	F	G	H	I	J
			_						
6448	OG ~	SER		141	26.615	10.552	18.225		23.99
6450	C	SER		141	27.456	8.023	16.856		22.90
6451	0	SER		141	28.248	7.250	17.390		22.85
6452	N	ASP		142	26.203	7.678	16.538		23.91
6454	CA	ASP		142	25.580	6.411	16.991		24.85
6456	CB	ASP		142	24.270	6.674	17.745		25.39
6459	CG	ASP		142	24.464	7.509	18.995		26.64
6460	OD1	ASP		142	23.535	8.249	19.365		25.98
6461	OD2	ASP		142	25.516	7.497	19.667	1.00	29.60
6462	C	ASP		142	25.262	5.407	15.890	1.00	25.42
6463	0	ASP		142	25.185	4.202	16.158	1.00	25.21
6464	N	ALA	В	143	25.052	5.887	14.663	1.00	25.69
6466	CA	ALA	В	143	24.533	5.031	13.592	1.00	26.20
6468	CB	ALA	В	143	24.187	5.840	12.367	1.00	26.13
6472	C	ALA	В	143	25.542	3.965	13.226	1.00	26.52
6473	0	ALA	В	143	26.739	4.190	13.292	1.00	26.08
6474	N	ASP	В	144	25.051	2.790	12.862	1.00	27.00
6476	CA	ASP	В	144	25.908	1.760	12.308	1.00	27.79
6478	CB	ASP	В	144	25.084	0.487	12.088	1.00	28.61
6481	CG	ASP	В	144	25.935	-0.733	11.853	1.00	30.23
6482	OD1	ASP	В	144	27.147	-0.714	12.160	1.00	33.26
6483	OD2	ASP	В	144	25.452	-1.776	11.358	1.00	34.68
6484	C	ASP	В	144	26.531	2.247	10.992	1.00	27.76
6485	0	ASP		144	25.825	2.652	10.050	1.00	27.93
6486	N	MET	В	145	27.856	2.247	10.951		27.25
6488	CA	MET	В	145	28.612	2.526	9.743	1.00	27.33
6490	CB	MET	В	145	29.181	3.936	9.772		26.88
6493	CG	MET	В	145	28.129	5.014	9.664		26.79
6496	SD	MET	В	145	28.859	6.646	9.270	1.00	27.26
6497	CE	MET	В	145	29.830	6.916	10.701		23.05
6501	С	MET	В	145	29.737	1.508	9.657		27.62
6502	0	MET	В	145	30.895	1.812	9.936	1.00	26.26
6503	N	PRO	В	146	29.393	0.291	9.256	1.00	
6504	CA	PRO	В	146	30.354	-0.815	9.234	1.00	29.73
6506	CB	PRO	В	146	29.669	-1.832	8.320	1.00	
6509	CG	PRO	В	146	28.228	-1.630	8.593	1.00	
6512	CD	PRO	В	146	28.060	-0.137	8.799		29.11
6515	С	PRO	В	146	31.733	-0.464	8.696		30.46
6516	0	PRO		146	32.732	-0.822	9.317		30.83
6517	N	GLU		147	31.801	0.253	7.586		31.81
6519	CA	GLU		147	33.089	0.431	6.905		33.36
6521	CB	GLU		147	32.889	0.840	5.426		34.57
6524	CG	GLU		147	31.629	0.304	4.730		37.40
6527	CD	GLU		147	31.768	0.264	3.209	1.00	
6528	OE1	GLU		147	30.918	-0.387	2.543	1.00	
6529	OE2	GLU		147	32.733	0.877	2.676	1.00	
6530	С	GLU		147	34.030	1.449	7.587	1.00	
6531	0	GLU		147	35.172	1.605	7.155		33.17
6532	N	VAL		148	33.572	2.099	8.660		31.25
6534	CA	VAL		148	34.097	3.410	9.043		30.18
6536	CB	VAL		148	32.970	4.456	9.012		30.21
6538		VAL		148	33.501	5.842	9.381		29.95

FIGURE 3 (Cont.)CL

A	В	С	D	E	F	G	Н	I	J
6542	CG2	VAL	В	148	32.310	4.467	7.634	1.00	30.63
6546	С	VAL		148	34.767	3.425	10.417		28.89
6547	0	VAL		148	34.131	3.174	11.431		27.43
6548	N	SER		149	36.057	3.755	10.435	1.00	28.02
6550	CA	SER	В	149	36.806	3.836	11.681	1.00	27.32
6552	СВ	SER	В	149	38.302	4.022	11.413	1.00	
6555	OG	SER	В	149	38.554	5.276	10.811	1.00	
6557	С	SER	В	149	36.295	4.984	12.540	1.00	27.03
6558	0	SER	В	149	35.651	5.906	12.045	1.00	26.50
6559	N	ASP	В	150	36.601	4.899	13.831	1.00	26.71
6561	CA	ASP	В	150	36.236	5.914	14.810	1.00	26.65
6563	CB	ASP	В	150	36.729	5.509	16.194	1.00	26.35
6566	CG	ASP	В	150	35.776	4.575	16.906	1.00	28.03
6567	OD1	ASP	В	150	36.086	4.216	18.054	1.00	30.17
6568		ASP		150	34.692	4.157	16.424	1.00	29.62
6569	С	ASP	В	150	36.824	7.253	14.407	1.00	26.23
6570	0	ASP		150	36.146	8.269	14.454	1.00	25.29
6571	N	ARG		151	38.077	7.229	13.970	1.00	26.28
6573	CA	ARG		151	38.745	8.409	13.442	1.00	26.55
6575	CB	ARG		151	40.172	8.069	13.019	1.00	
6578	CG	ARG		151	41.099	9.254	13.054	1.00	30.78
6581	CD	ARG		151	41.726	9.500	14.416	1.00	
6584	NE	ARG		151	41.001	10.520	15.179	1.00	38.97
6586	CZ	ARG		151	41.152	11.835	15.043	1.00	
6587	NH1	ARG		151	42.000	12.354	14.148	1.00	45.06
6590	NH2	ARG		151	40.435	12.651	15.801	1.00	43.15
6593	C	ARG		151	38.004	9.052	12.268	1.00	
6594	0	ARG		151	37.870	10.265	12.211	1.00	
6595	N	ASP	В	152	37.540	8.252	11.315	1.00	
6597	CA	ASP	В	152	36.823	8.813	10.171	1.00	
6599 6602	CB CG	ASP ASP	В	152	36.747	7.809	9.030	1.00	
6603	OD1	ASP		152	38.117	7.499	8.443	1.00	
6604		ASP	B B	152 152	39.074	8.280 6.479	8.679 7.758		29.38
6605	C	ASP		152	38.329 35.427	9.290	10.562		28.43 22.75
6606	0	ASP		152	34.923	10.240	10.362	1.00	
6607	N	ARG		153	34.810	8.619	11.521		21.86
6609	CA	ARG		153	33.532	9.053	12.064		20.79
6611	СВ	ARG		153	33.022	8.054	13.088		20.73
6614	CG	ARG		153	31.647	8.375	13.651		20.82
6617	CD	ARG		153	31.205	7.399	14.704		20.94
6620	NE	ARG		153	30.980	6.045	14.173		22.48
6622	CZ	ARG		153	29.790	5.511	13.895		23.71
6623		ARG		153	29.723	4.256	13.448		25.23
6626		ARG		153	28.671	6.205	14.046		20.67
6629	С	ARG		153	33.676	10.426	12.714	1.00	
6630	0	ARG		153	32.833	11.297	12.519	1.00	
6631	N	ILE		154	34.752	10.610	13.483	1.00	
6633	CA	ILE		154	35.016	11.891	14.124		20.38
6635	CB	ILE	В	154	36.209	11.808	15.090		20.21
6637	CG1	ILE		154	35.848	10.962	16.319		20.02
6640	CD1	ILE	В	154	37.077	10.390	17.035	1.00	21.78

FIGURE 3 (Cont.)CM

A	В	С	D	Е	F	G	Н	I	J
6644	CG2	ILE	В	154	36.656	13.203	15.514	1.00	21.46
6648	C	ILE		154	35.247	12.940	13.051		20.53
6649	0	ILE		154	34.737	14.018	13.158		20.41
6650	N	SER		155	35.976	12.593	11.996		21.07
6652	CA	SER		155	36.182	13.485	10.864	1.00	21.78
6654	СВ	SER		155	37.097	12.822	9.824	1.00	22.36
6657	OG	SER		155	38.452	13.117	10.107	1.00	25.91
6659	C	SER		155	34.867	13.924	10.186		21.46
6660	Ō	SER		155	34.771	15.053	9.711		21.56
6661	N	MET	В	156	33.886	13.029	10.125		21.47
6663	CA	MET	В	156	32.569	13.337	9.576	1.00	21.23
6665	СВ	MET	В	156	31.726	12.079	9.403	1.00	21.94
6668	CG		В	156	32.183	11.183	8.281		24.79
6671	SD	MET		156	31.189	9.677	8.224	1.00	31.73
6672	CE	MET		156	32.337	8.674	7.553	1.00	32.04
6676	С		В	156	31.815	14.278	10.480	1.00	20.18
6677	0		В	156	31.164	15.191	10.005	1.00	20.12
6678	N	ILE		157	31.894	14.045	11.782	1.00	20.00
6680	CA	ILE	В	157	31.238	14.915	12.744	1.00	19.69
6682	СВ	ILE	В	157	31.290	14.326	14.178	1.00	19.62
6684	CG1	ILE	В	157 ·	30.466	13.047	14.259	1.00	19.47
6687	CD1	ILE	В	157	30.741	12.182	15.483	1.00	21.29
6691	CG2	ILE	В	157	30.763	15.332	15.177	1.00	18.69
6695	С	ILE	В	157	31.878	16.289	12.688	1.00	19.80
6696	0	ILE	В	157	31.182	17.300	12.684	1.00	20.00
6697	N	SER	В	158	33.204	16.340	12.640	1.00	19.73
6699	CA	SER	В	158	33.894	17.619	12.559	1.00	19.44
6701	CB	SER	В	158	35.410	17.419	12.507	1.00	19.53
6704	OG	SER	В	158	36.053	18.665	12.347	1.00	19.74
6706	С	SER	В	158	33.469	18.403	11.325	1.00	19.46
6707	0	SER	В	158	33.193	19.587	11.408	1.00	18.61
6708	N	GLU	В	159	33.429	17.734	10.181	1.00	20.02
6710	CA	GLU	В	159	33.084	18.384	8.932	1.00	20.06
6712	CB	GLU	В	159	33.224	17.423	7.757	1.00	20.49
6715	CG	GLU	В	159	32.576	17.922	6.472	1.00	21.89
6718	CD	GLU		159	33.103	19.290	6.041	1.00	23.61
6719	OE1	GLU		159	34.281	19.584	6.322		24.99
6720	OE2	GLU		159	32.347	20.067	5.426		25.28
6721	С	GLU		159	31.658	18.934	8.990		19.72
6722	0	GLU		159	31.422	20.062	8.577		19.69
6723	N	LEU		160	30.720	18.140	9.494		18.90
6725	CA	LEU		160	29.324	18.550	9.526	1.00	18.94
6727	CB	LEU		160	28.406	17.404	9.956	1.00	
6730	CG	LEU		160	26.915	17.695	9.771		19.53
6732	CD1	LEU		160	26.644	18.166	8.357		19.83
6736	CD2	LEU		160	26.076	16.470	10.093		20.63
6740	C	LEU		160	29.158	19.736	10.458	1.00	
6741	0	LEU		160	28.486	20.694	10.130	1.00	
6742	N	ALA		161	29.803	19.673	11.612	1.00	
6744	CA	ALA		161	29.769	20.773	12.560	1.00	18.51
6746	CB	ALA		161	30.446	20.384	13.872	1.00	18.21
6750	С	ALA	B	161	30.377	22.045	11.970	1.00	19.04

FIGURE 3 (Cont.)CN

A	В	С	D	E	F	G	Н	I	J
6751	0	ALA	В	161	29.749	23.095	12.012	1.00	18.97
6752	N	SER		162	31.573	21.976	11.387	1.00	19.49
6754	CA	SER		162	32.161	23.190	10.838	1.00	19.97
6756	CB	SER		162	33.630	22.988	10.472		20.60
6759	OG	SER	В	162	33.756	21.975	9.518	1.00	24.18
6761	С	SER	В	162	31.348	23.734	9.643	1.00	19.40
6762	0	SER	В	162	31.186	24.958	9.482	1.00	18.70
6763	N	ALA	В	163	30.813	22.832	8.825	1.00	19.19
6765	CA	ALA	В	163	29.974	23.225	7.690	1.00	18.98
6767	CB	ALA	В	163	29.671	22.011	6.798	1.00	19.19
6771	C	ALA	В	163	28.672	23.907	8.081	1.00	18.85
6772	0	ALA	В	163	28.157	24.742	7.341	1.00	19.30
6773	N	SER	В	164	28.135	23.537	9.228	1.00	18.81
6775	CA	SER	В	164	26.788	23.931	9.638	1.00	18.52
6777	CB	SER	В	164	26.128	22.787	10.405	1.00	18.45
6780	OG	SER		164	26.073	21.610	9.622	1.00	18.06
6782	С	SER		164	26.780	25.159	10.526	1.00	18.48
6783	0	SER		164	25.779	25.828	10.630	1.00	18.20
6784	N	GLY		165	27.902	25.438	11.177	1.00	19.42
6786	CA	GLY		165	27.950	26.481	12.175	1.00	19.70
6789	C	GLY		165	28.359	27.810	11.598	1.00	
6790	0	GLY		165	28.096	28.122	10.441	1.00	19.41
6791	N	ILE		166	29.018	28.604	12.424	1.00	21.45
6793	CA	ILE		166	29.348	29.976	12.074	1.00	22.91
6795	CB	ILE		166	29.846	30.707	13.354	1.00	23.50
6797	CG1	ILE		166	29.737	32.206	13.173		25.77
6800	CD1	ILE		166	28.314	32.688	13.353	1.00	25.49
6804	CG2	ILE		166	31.229	30.245	13.727	1.00	24.89
6808	C	ILE		166	30.354	30.068	10.916	1.00	22.56
6809	0	ILE		166	30.335	31.016	10.141	1.00	22.77
6810	N	ALA		167	31.207	29.059	10.771	1.00	
6812 6814	CA CB	ALA ALA		167	32.152 33.324	29.006	9.656	1.00	22.06
6818	СВ	ALA		167 167	31.490	28.148 28.488	10.023	1.00	21.92
6819	0	ALA		167	32.146	28.488	8.383	1.00	22.04
6820	N	GLY		168	30.181	28.252	7.376 8.430	1.00	21.24
6822	CA	GLY		168	29.464	27.684	7.313	1.00	20.53
6825	C	GLY		168	28.034	28.189	7.292	-	20.28
6826	o	GLY		168	27.804	29.394	7.295		19.03
6827	N	MET		169	27.082	27.265	7.340		20.39
6829	CA	MET		169	25.676	27.559	7.077		21.14
6831	СВ	MET		169	24.855	26.298	7.278		21.40
6834	CG	MET		169	23.410	26.392	6.837		23.14
6837	SD	MET		169	22.401	27.153	8.090		26.74
6838	CE	MET		169	22.407	25.862	9.410		26.17
6842	С	MET		169	25.147	28.696	7.938		21.67
6843	0	MET	В	169	24.556	29.644	7.436		21.21
6844	N	CYS		170	25.367	28.594	9.239		22.13
6846	CA	CYS		170	24.827	29.556	10.170		22.50
6848	CB I	BCYS	В	170	25.042	29.096	11.614		22.49
6849		ACYS		170	25.010	29.057	11.596	0.65	22.96
6854	SG I	BCYS	В	170	23.609	28.307	12.340	0.35	22.05

FIGURE 3 (Cont.)CO

A	В	С	D	E	F	G	Н	I	J
6855	SG	ACYS	В	170	24.028	29.996	12.749	0.65	25.42
6856	C	CYS		170	25.460	30.935	9.997	1.00	21.94
6857	0	CYS		170	24.775	31.934	10.105	1.00	22.08
6858	N	GLY		171	26.767	30.980	9.758	1.00	21.27
6860	CA	GLY	В	171	27.453	32.231	9.504	1.00	21.35
6863	С	GLY	В	171	26.951	32.858	8.218	1.00	20.97
6864	0	GLY	В	171	26.839	34.081	8.111	1.00	20.81
6865	N	GLY	В	172	26.643	32.009	7.249	1.00	20.08
6867	CA	GLY	В	172	26.027	32.440	6.009	1.00	19.62
6870	C	GLY	В	172	24.641	33.007	6.215	1.00	19.25
6871	0	GLY		172	24.288	34.011	5.605	1.00	18.27
6872	N	GLN		173	23.858	32.380	7.084	1.00	18.75
6874	CA	GLN		173	22.535	32.890	7.404	1.00	19.22
6876	CB	GLN		173	21.787	31.947	8.348	1.00	19.67
6879	CG	GLN		173	21.349	30.652	7.682	1.00	20.18
6882	CD	GLN		173	20.333	30.899	6.597	1.00	20.92
6883	OE1			173	20.701	31.297	5.496	1.00	21.77
6884	NE2			173	19.047	30.712	6.914	1.00	19.90
6887	C	GLN		173	22.632	34.281	8.002	1.00	19.31
6888	0	GLN		173	21.805	35.146	7.691	1.00	18.98
6889	N Ca	ALA		174	23.667	34.503	8.810	1.00	19.26
6891 6893	CA CB	ALA ALA		174 174	23.894 24.956	35.813 35.725	9.437	1.00	20.09
6897	C	ALA		174	24.336	36.845	10.526 8.387	1.00	19.57 20.47
6898	0	ALA		174	23.826	37.969	8.440	1.00	21.60
6899	N	LEU		175	25.143	36.464	7.436	1.00	21.00
6901	CA	LEU		175	25.561	37.384	6.371	1.00	21.21
6903	CB	LEU		175	26.646	36.753	5.497	1.00	21.41
6906	CG	LEU		175	28.026	36.557	6.121	1.00	23.45
6908	CD1	LEU	В	175	28.948	35.855	5.138	1.00	24.47
6912	CD2	LEU	В	175	28.630	37.913	6.562	1.00	24.78
6916	C	LEU	В	175	24.358	37.776	5.519	1.00	21.36
6917	0	LEU	В	175	24.210	38.942	5.118	1.00	20.88
6918	N	ASP	В	176	23.498	36.794	5.258	1.00	21.82
6920	CA		В	176	22.291	36.980	4.466	1.00	22.30
6922	CB		В	176	21.615	35.625	4.252	1.00	22.47
6925	CG		В	176	20.205	35.739	3.779		21.57
6926		ASP		176	19.938	35.449	2.588	1.00	
6927		ASP		176	19.281	36.072	4.540	1.00	
6928	C	ASP		176	21.356	37.989	5.138	1.00	23.38
6929 6930	O N	ASP		176	20.856	38.927	4.499	1.00	23.61
6932	CA	LEU LEU		177 177	21.131 20.296	37.814 38.751	6.429 7.181	1.00	24.61
6934	CB	LEU		177	20.236	38.267	8.621	1.00	26.08 26.86
6937	CG	LEU		177	18.842	37.475	8.968	1.00	
6939		LEU		177	18.029	36.990	7.768	1.00	
6943	CD2	LEU		177	19.243	36.330	9.825	1.00	29.29
6947	C	LEU		177	20.891	40.147	7.193	1.00	26.38
6948	Ō	LEU		177	20.176	41.134	7.048		27.18
6949	N	ASP		178	22.203	40.228	7.355		27.07
6951	CA	ASP	В	178	22.893	41.513	7.389		27.97
6953	CB	ASP	В	178	24.336	41.337	7.864	1.00	28.49

FIGURE 3 (Cont.)CP

A	В	С	D	E	F	G	Н	I	J
6956	CG	ASP	В	178	24.926	42.624	8.427	1.00	31.55
6957	OD1			178	25.937	43.106	7.874	1.00	34.43
6958	OD2	ASP		178	24.447	43.218	9.419	1.00	36.43
6959	С	ASP		178	22.865	42.228	6.034	1.00	27.98
6960	0	ASP		178	22.853	43.454	5.993	1.00	27.47
6961	N	ALA		179	22.828	41.462	4.936	1.00	27.64
6963	CA	ALA	В	179	22.818	42.026	3.576	1.00	27.64
6965	CB	ALA	В	179	23.397	41.024	2.579	1.00	27.26
6969	C	ALA	В	179	21.415	42.474	3.118	1.00	27.90
6970	0	ALA	В	179	21.288	43.142	2.109	1.00	27.38
6971	N	GLU	В	180	20.374	42.097	3.852	1.00	28.50
6973	CA	GLU	В	180	19.006	42.515	3.535	1.00	29.13
6975	CB	GLU	В	180	18.031	42.069	4.629	1.00	29.71
6978	CG	GLU	В	180	17.071	40.969	4.234	1.00	31.66
6981	CD	GLU		180	16.175	40.534	5.384	1.00	33.14
6982	OE1	GLU		180	15.509	41.400	5.995	1.00	35.30
6983	OE2	GLU		180	16.149	39.324	5.684	1.00	32.62
6984	С	GLU		180	18.922	44.041	3.418	1.00	29.49
6985	0	GLU		180	19.290	44.755	4.348	1.00	28.60
6986	N	GLY		181	18.454	44.518	2.264	1.00	
6988	CA	GLY		181	18.279	45.935	1.997	1.00	29.83
6991	C	GLY		181	19.560	46.670	1.658	1.00	
6992	0	GLY		181	19.532	47.871	1.420	1.00	
6993	N	LYS		182	20.681	45.954	1.622	1.00	30.21
6995	CA		В	182	21.992	46.573	1.506	1.00	30.46
6997	CB	LYS	В	182	22.959	45.982	2.526	1.00	30.97
7000	CG	LYS	В	182	22.593	46.287	3.973	1.00	32.58
7003	CD	LYS	В	182	23.830	46.343	4.864	1.00	34.32
7006 7009	CE NZ	LYS LYS		182 182	23.490	46.882 45.804	6.259	1.00	35.98
7013	C	LYS	В	182	23.339 22.573	46.427	7.290 0.116	1.00	36.88 30.22
7013	0	LYS		182	23.559	47.083	-0.203	1.00	30.22
7015	N	HIS		183	21.984	45.555	-0.700	1.00	29.28
7017	CA	HIS		183	22.375	45.441	-2.093	1.00	
7019	СВ	HIS	В	183	21.892	46.684	-2.856	1.00	29.70
7022	CG	HIS	В	183	20.410	46.833	-2.832	1.00	30.08
7023	ND1	HIS	В	183	19.699	47.003	-1.668	1.00	32.28
7025		HIS	В	183	18.412	47.068	-1.942		31.16
7027		HIS		183	18.261	46.940	-3.244		32.50
7029		HIS		183	19.497	46.782	-3.821		32.70
7031	C	HIS	В	183	23.887	45.297	-2.191	1.00	28.93
7032	0	HIS	В	183	24.558	46.097	-2.847		29.19
7033	N	VAL	В	184	24.415	44.274	-1.522	1.00	27.85
7035	CA	VAL	В	184	25.850	44.103	-1.417	1.00	27.29
7037	CB	VAL		184	26.247	43.065	-0.319		27.33
7039		VAL		184	25.636	43.452	1.052		27.10
7043	CG2			184	25.860	41.634	-0.722		27.05
7047	C	VAL		184	26.419	43.723	-2.779		26.86
7048	0	VAL		184	25.733	43.075	-3.577		26.12
7049	N	PRO		185	27.663	44.126	-3.051		26.31
7050	CA	PRO		185	28.314	43.792	-4.319		26.16
7052	CB	PRO	B	185	29.596	44.623	-4.284	T.00	26.24

FIGURE 3 (Cont.)CQ

Α	В	С	D	E	F	G	H	I	J
7055	~~	nno	_	105	20 002	44 001	0 005		06.65
7055	CG	PRO		185	29.892	44.801	-2.835		26.65
7058	CD	PRO		185	28.552	44.905	-2.168		26.81
7061	C	PRO		185	28.646	42.297	-4.436	1.00	25.85
7062	0	PRO		185	28.521	41.553	-3.475	1.00	
7063	N	LEU		186	29.106	41.908	-5.616		26.22
7065	CA	LEU		186	29.284	40.509	-6.002	1.00	
7067	CB	LEU		186	29.859	40.422	-7.424	1.00	
7070	CG	LEU		186	29.462	39.279	-8.371	1.00	28.07
7072	CD1	LEU		186	30.565	39.033	-9.399		29.61
7076 7080	CD2 C	LEU LEU		186 186	29.105	38.004	-7.671		28.33
7081	0	LEU		186	30.183	39.726	-5.048		26.27
7081	N	ASP		187	29.890	38.580	-4.737		25.80
7082	CA	ASP		187	31.286	40.317	-4.590	1.00	
7084	CB	ASP		187	32.198 33.567	39.558 40.236	-3.721	1.00	27.11
7089	CG	ASP		187	33.480	41.648	-3.526 -2.951	1.00	27.85 30.82
7090	OD1	ASP		187	34.555	42.173	-2.574	1.00	
7091	OD2	ASP		187	32.435	42.331	-2.848	1.00	35.53
7092	C	ASP		187	31.554	39.180	-2.380	1.00	26.24
7093	0	ASP		187	31.729	38.053	-1.900		25.65
7094	N	ALA		188	30.809	40.117	-1.799		25.42
7096	CA	ALA		188	30.003	39.892	-0.548		24.85
7098	CB	ALA		188	29.610	41.221	0.019		24.84
7102	C	ALA		188	28.915	38.951	-0.774	1.00	
7103	0	ALA		188	28.578	38.154	0.081	1.00	
7104	N	LEU		189	28.291	39.059	-1.942	1.00	
7106	CA	LEU		189	27.156	38.230	-2.286	1.00	
7108	CB	LEU		189	26.530	38.741	-3.577	1.00	24.99
7111	CG	LEU		189	25.509	37.865	-4.268	1.00	25.94
7113	CD1	LEU	В	189	24.317	37.593	-3.350	1.00	26.65
7117	CD2	LEU	В	189	25.072	38.566	-5.566		26.30
7121	С	LEU	В	189	27.607	36.783	-2.435	1.00	23.85
7122	0	LEU	В	189	26.965	35.863	-1.918	1.00	23.56
7123	N	GLU	В	190	28.727	36.590	-3.115	1.00	23.22
7125	CA	GLU	В	190	29.301	35.269	-3.280	1.00	23.29
7127	CB	GLU	В	190	30.566	35.331	-4.135	1.00	23.75
7130	CG	GLU	В	190	31.070	33.963	-4.535	1.00	25.63
7133	CD	GLU		190	32.356	33.994	-5.339		28.46
7134		GLU		190	33.201	33.121	-5.090		31.64
7135		GLU		190	32.522	34.854	-6.226		32.12
7136	С	GLU		190	29.625	34.655	-1.917		22.85
7137	0	GLU		190	29.434	33.459	-1.699		20.62
7138	N	ARG		191	30.114	35.490	-1.009		22.57
7140	CA	ARG		191	30.499	35.041	0.315		22.97
7142	CB	ARG		191	31.169	36.171	1.077		23.59
7145	CG	ARG		191	31.646	35.789	2.444		26.56
7148	CD	ARG		191	32.707	36.714	3.004		31.42
7151	NE	ARG		191	32.158	37.666	3.962		35.82
7153	CZ	ARG		191	32.874	38.304	4.891		38.83
7154	NH1			191 191	34.184	38.105	5.012		39.90
7157 7160	NH2 C	ARG ARG		191 191	32.270 29.282	39.150 34.546	5.712 1.087		40.92
1100		AAG	D	エフエ	43.404	34.340	1.00/	1.00	21.94

FIGURE 3 (Cont.)CR

Α	В	С	D	E	F	G	H	I	J
	_		_						
7161	0	ARG		191	29.357	33.536	1.770	1.00	
7162	N	ILE		192	28.160	35.246	0.947	1.00	
7164	CA	ILE		192	26.916	34.836	1.574	1.00	
7166	CB	ILE		192	25.763	35.775	1.186	1.00	
7168	CG1	ILE		192	25.925	37.151	1.835	1.00	
7171	CD1	ILE		192	25.092	38.196	1.195	1.00	
7175	CG2	ILE		192	24.408	35.196	1.598	1.00	
7179	C	ILE		192	26.589	33.421	1.107	1.00	
7180 7181	N O		В	192	26.387	32.538	1.914	1.00	
7181	CA	HIS HIS	В	193 193	26.542	33.231 31.999	-0.207	1.00	
7185	CB	HIS		193	26.027		-0.802	1.00	
7188	CG	HIS		193	25.801 24.584	32.209	-2.298	1.00	
7189			В	193	23.920	33.024	-2.606	1.00	
7191		HIS	В	193	22.873	33.755	-1.647 -2.191	1.00	
7193	NE2	HIS	В	193	22.873	34.349 34.013		1.00	
7195			В	193	23.882	33.186	-3.467 -3.754	1.00	19.16 19.39
7197	C	HIS		193	26.913	30.802			
7198	0	HIS		193	26.422	29.700	-0.543 -0.294	1.00	18.45
7199	N	ARG		194	28.221	31.017	-0.294	1.00	18.16
7201	CA	ARG		194	29.157	29.954	-0.301	1.00	18.21
7203	CB	ARG		194	30.582	30.396	-0.588	1.00	18.14 18.28
7206	CG	ARG		194	30.894	30.549	-2.059	1.00	
7209	CD	ARG		194	32.368	30.549	-2.332	1.00	18.14 19.86
7212	NE	ARG		194	32.685	30.696	-2.332	1.00	20.51
7214	CZ	ARG		194	32.656	29.723	-4.648	1.00	
7215	NH1	ARG		194	32.326	28.482	-4.320	1.00	23.08 24.68
7218	NH2	ARG		194	32.981	29.995	-5.900	1.00	
7221	C	ARG		194	29.003	29.465	1.143	1.00	18.28
7222	ō	ARG		194	29.037	28.267	1.392	1.00	18.15
7223	N	HIS		195	28.782	30.390	2.079	1.00	18.49
7225	CA	HIS		195	28.558	30.036	3.479	1.00	18.76
7227	СВ	HIS		195	28.786	31.251	4.390	1.00	18.80
7230	CG	HIS		195	30.224	31.612	4.533	1.00	19.89
7231		HIS		195	30.934	32.241	3.533	1.00	
7233		HIS		195	32.186	32.408	3.925	1.00	
7235		HIS		195	32.311	31.910	5.142	1.00	
7237	CD2	HIS	В	195	31.103	31.395	5.541	1.00	21.40
7239	C	HIS	В	195	27.170	29.430	3.697	1.00	
7240	0	HIS	В	195	27.050	28.298	4.182	1.00	19.41
7241	N	LYS	В	196	26.117	30.122	3.293	1.00	18.32
7243	CA	LYS	В	196	24.778	29.672	3.686	1.00	18.29
7245	CB	LYS	В	196	23.725	30.764	3.506	1.00	18.11
7248	CG	LYS	В	196	23.241	31.027	2.080	1.00	17.45
7251	CD	LYS	В	196	22.081	32.049	2.131	1.00	17.15
7254	CE	LYS	В	196	21.634	32.547	0.768	1.00	15.61
7257	NZ	LYS		196	20.235	33.122	0.794	1.00	15.01
7261	С	LYS		196	24.322	28.389	3.006	1.00	18.44
7262	0	LYS		196	23.466	27.688	3.541	1.00	18.43
7263	N	THR		197	24.898	28.098	1.841	1.00	17.92
7265	CA	THR		197	24.454	27.009	0.983	1.00	18.22
7267	CB	THR	В	197	23.686	27.598	-0.203	1.00	17.81

FIGURE 3 (Cont.)CS

A	В	С	D	E	F	G	Н	I	J
7269	OG1	THR	В	197	22.429	28.070	0.261	1.00	18.26
7271	CG2	THR		197	23.322	26.539	-1.246	1.00	18.58
7275	C	THR		197	25.601	26.129	0.504	1.00	17.84
7276	o	THR		197	25.482	24.907	0.475	1.00	18.55
7277	N	GLY		198	26.703	26.746	0.104	1.00	17.60
7279	CA	GLY		198	27.854	26.006	-0.358	1.00	17.04
7282	C	GLY		198	28.469	25.112	0.708	1.00	16.72
7283	0	GLY		198	28.863	23.112	0.708	1.00	15.65
7284	N	ALA		199	28.523	25.581	1.951	1.00	
7286	CA	ALA		199	29.239	24.837	2.993	1.00	16.19
7288	CB	ALA		199	29.265	25.611			16.23
7292	С	ALA		199		23.441	4.271	1.00	16.00
7293	0	ALA			28.633		3.200	1.00	16.09
7294	N	LEU		199 200	29.357	22.445	3.312	1.00	16.00
7296	CA	LEU			27.309	23.363	3.200	1.00	15.80
				200	26.623	22.126	3.536	1.00	16.20
7298	CB	LEU		200	25.202	22.408	4.018	1.00	16.05
7301	CG	LEU		200	24.363	21.238	4.540	1.00	18.16
7303	CD1	LEU		200	25.019	20.573	5.727	1.00	18.85
7307	CD2	LEU		200	22.989	21.735	4.928	1.00	18.03
7311	C	LEU		200	26.593	21.206	2.332	1.00	16.19
7312	0	LEU		200	26.544	19.993	2.479	1.00	15.79
7313	N	ILE		201	26.615	21.769	1.136	1.00	16.74
7315	CA	ILE		201	26.723	20.928	-0.052	1.00	17.10
7317	CB	ILE		201	26.341	21.713	-1.305	1.00	17.41
7319	CG1		В	201	24.806	21.764	-1.403	1.00	18.09
7322	CD1	ILE		201	24.283	22.985	-2.120	1.00	19.65
7326	CG2	ILE		201	26.936	21.073	-2.581	1.00	16.41
7330	C	ILE		201	28.130	20.312	-0.110	1.00	17.27
7331	0	ILE		201	28.289	19.126	-0.436	1.00	16.47
7332	N	ARG		202	29.139	21.098	0.240	1.00	17.03
7334	CA	ARG		202	30.468	20.539	0.389	1.00	17.33
7336	CB	ARG		202	31.516	21.598	0.645	1.00	17.65
7339	CG	ARG		202	32.956	20.997	0.625	1.00	18.08
7342	CD	ARG		202	34.038	22.029	0.637	1.00	19.46
7345	NE	ARG		202	33.985	22.829	1.854	1.00	21.33
7347	CZ	ARG		202	34.772	23.882	2.089	1.00	22.51
7348	NH1	ARG		202	34.662	24.547	3.222	1.00	23.90
7351		ARG		202	35.663	24.271	1.199		21.54
7354	С	ARG		202	30.517	19.475	1.475		17.44
7355	0	ARG		202	31.179	18.451	1.295	1.00	
7356	N	ALA		203	29.804	19.689	2.580	1.00	
7358	CA	ALA		203	29.776	18.709	3.658	1.00	
7360	СВ	ALA		203	28.967	19.200	4.832		17.56
7364	С	ALA		203	29.211	17.389	3.179	1.00	17.03
7365	0	ALA		203	29.704	16.351	3.574	1.00	15.70
7366	N	ALA		204	28.154	17.439	2.368	1.00	16.79
7368	CA	ALA		204	27.548	16.224	1.799	1.00	17.41
7370	СВ	ALA		204	26.386	16.572	0.915	1.00	17.51
7374	С	ALA		204	28.560	15.419	1.002	1.00	17.70
7375	O N	ALA		204	28.698	14.197	1.200	1.00	17.88
7376	N	VAL		205	29.268	16.107	0.109	1.00	17.07
7378	CA	VAL	Þ	205	30.282	15.471	-0.724	1.00	17.54

FIGURE 3 (Cont.)CT

A	В	С	D	E	F	G	Н	I	J
7380	СВ	VAL	В	205	30.849	16.429	-1.793	1.00	17.01
7382	CG1	VAL		205	31.962	15.769	-2.607	1.00	17.61
7386	CG2	VAL	В	205	29.750	16.884	-2.730	1.00	17.80
7390	C	VAL		205	31.400	14.924	0.150	1.00	18.04
7391	0	VAL		205	31.802	13.766	-0.005	1.00	17.71
7392	N	ARG		206	31.887	15.748	1.078	1.00	18.26
7394	CA	ARG		206	32.974	15.348	1.963	1.00	18.54
7396	CB	ARG		206	33.393	16.497	2.878	1.00	19.04
7399	CG	ARG		206	34.211	17.532	2.179	1.00	18.96
7402	CD	ARG	В	206	34.665	18.637	3.113	1.00	20.46
7405	NE	ARG	В	206	35.712	19.448	2.531	1.00	20.99
7407	CZ	ARG	В	206	36.218	20.545	3.102	1.00	21.01
7408	NH1	ARG	В	206	35.771	20.974	4.275	1.00	20.38
7411	NH2	ARG	В	206	37.190	21.204	2.495	1.00	20.62
7414	С	ARG	В	206	32.582	14.152	2.795	1.00	18.87
7415	0	ARG	В	206	33.368	13.219	2.935	1.00	18.67
7416	N	LEU	В	207	31.346	14.136	3.289	1.00	19.33
7418	CA	LEU	В	207	30.896	13.036	4.141	1.00	20.12
7420	CB	LEU	В	207	29.516	13.310	4.738	1.00	19.99
7423	CG	LEU	В	207	29.431	13.776	6.203	1.00	22.44
7425	CD1	LEU		207	30.464	14.770	6.559	1.00	24.69
7429	CD2	LEU		207	28.046	14.364	6.440	1.00	24.61
7433	С	LEU		207	30.887	11.715	3.370	1.00	20.21
7434	0	LEU		207	31.247	10.668	3.922	1.00	20.74
7435	N	GLY		208	30.461	11.750	2.110	1.00	20.90
7437	CA	GLY		208	30.546	10.578	1.246	1.00	21.11
7440	С	GLY		208	31.979	10.097	1.066	1.00	21.83
7441	0	GLY		208	32.263	8.898	1.152	1.00	22.91
7442	N	ALA		209	32.892	11.029	0.821	1.00	21.98
7444	CA	ALA		209	34.292	10.688	0.627	1.00	22.48
7446	CB	ALA		209	35.059	11.868	0.052	1.00	22.44
7450	С О	ALA ALA		209	34.934	10.189	1.928	1.00	23.19
7451 7452	N	LEU		209 210	35.703 34.582	9.232 10.804	1.906 3.058	1.00	23.21
7454	CA	LEU		210	35.144	10.429	4.355	1.00	23.38
7454	CB	LEU		210	34.733	11.429	5.440	1.00	23.69
7459	CG	LEU		210	35.459	12.768	5.355	1.00	23.52
7461		LEU		210	34.830	13.745	6.336		22.14
7465		LEU		210	36.962	12.569	5.630		24.32
7469	С	LEU		210	34.721	9.031	4.780		24.42
7470	0	LEU		210	35.379	8.410	5.603		24.38
7471	N	SER		211	33.627	8.541	4.211		25.75
7473	CA	SER		211	33.176	7.180	4.458		26.29
7475	CB I	BSER		211	31.724	6.990	3.992	0.35	
7476	CB Z	ASER	В	211	31.733	7.003	3.960	0.65	
7481		BSER		211	31.635	6.814	2.589	0.35	
7482	OG I	ASER	В	211	30.884	8.043	4.437		28.22
7485	С	SER	В	211	34.096	6.146	3.779	1.00	26.79
7486	0	SER		211	33.943	4.960	4.011		27.11
7487	N	ALA		212	35.052	6.609	2.971		27.48
7489	CA	ALA		212	35.807	5.765	2.045		28.00
7491	CB	ALA	В	212	35.502	6.200	0.610	1.00	27.64

FIGURE 3 (Cont.)CU

A	В	С	D	E	F	G	Н	I	J
7495	С	ALA	В	212	37.330	5.735	2.259	1.00	28.36
7496	0	ALA	В	212	38.075	5.478	1.305	1.00	28.63
7497	N	GLY	В	213	37.793	6.017	3.480	1.00	28.63
7499	CA	GLY	В	213	39.190	5.812	3.848	1.00	28.66
7502	С	GLY		213	40.160	6.623	3.013	1.00	29.30
7503	0	GLY		213	39.829	7.754	2.628	1.00	29.18
7504	N	ASP		214	41.337	6.047	2.725	1.00	
7506	CA	ASP		214	42.401	6.716	1.945	1.00	
7508	СВ	ASP		214	43.629	5.798	1.749	1.00	31.13
7511	CG	ASP		214	44.248	5.315	3.055	1.00	32.74
7512	OD1	ASP		214	44.060	5.963	4.113	1.00	
7513	OD2	ASP		214	44.958	4.280	3.097	1.00	35.20
7514	С	ASP		214	41.960	7.157	0.541	1.00	
7515	0	ASP		214	42.333	8.224	0.068		29.72
7516	N	LYS		215	41.203	6.319	-0.150	1.00	30.05
7518	CA	LYS		215	40.854	6.614	-1.546	1.00	
7520	СВ	LYS		215	40.230	5.391	-2.199	1.00	30.71
7523	CG	LYS		215	40.214	5.394	-3.723	1.00	32.45
7526	CD		В	215	39.887	3.980	-4.222	1.00	
7529	CE	LYS		215	39.790	3.882	-5.732	1.00	36.80
7532	NZ	LYS		215	39.315	2.521	-6.190	1.00	38.07
7536	C	LYS		215	39.906	7.821	-1.634		28.89
7537	Ö	LYS		215	40.045	8.661	-2.525	1.00	28.45
7538	N	GLY		216	38.972	7.902	-0.689		27.81
7540	CA	GLY		216	38.049	9.018	-0.591	1.00	27.11
7543	C	GLY		216	38.781	10.292	-0.243	1.00	26.53
7544	0	GLY		216	38.559	11.333	-0.840	1.00	26.52
7545	N	ARG		217	39.690	10.198	0.720	1.00	26.28
7547	CA	ARG		217	40.519	11.340	1.099		25.74
7549	CB	ARG		217	41.263	11.018	2.393		25.35
7552	CG	ARG		217	40.332	11.005	3.598	1.00	28.38
7555	CD	ARG		217	40.945	10.453	4.857	1.00	31.47
7558	NE	ARG		217	40.208	10.787	6.078	1.00	33.37
7560	CZ	ARG		217	40.258	11.974	6.697	1.00	36.00
7561	NH1	ARG		217	40.977	12.979	6.200	1.00	39.28
7564	NH2	ARG		217	39.575	12.170	7.810	1.00	34.96
7567	С	ARG		217	41.471	11.800	-0.027		24.69
7568	0	ARG	В	217	41.743	12.983	-0.161		24.52
7569	N	ARG		218	41.956	10.873	-0.844		24.21
7571	CA	ARG		218	42.809	11.210	-1.983		23.79
7573	CB	ARG	В	218	43.340	9.927	-2.637		24.37
7576	CG	ARG		218	44.257	10.097	-3.872		27.47
7579	CD	ARG		218	43.908	9.115	-5.003		32.66
7582	NE	ARG	В	218	45.013	8.799	-5.908	1.00	
7584	CZ	ARG	В	218	45.406	9.552	-6.933	1.00	39.40
7585	NH1	ARG	В	218	46.425	9.145	-7.688	1.00	40.57
7588	NH2	ARG	В	218	44.809	10.714	-7.204	1.00	39.74
7591	С	ARG	В	218	42.025	12.047	-3.005		22.91
7592	0	ARG	В	218	42.599	12.928	-3.640		22.18
7593	N	ALA		219	40.726	11.759	-3.149	1.00	21.70
7595	CA	ALA	В	219	39.845	12.476	-4.066	1.00	21.49
7597	CB	ALA	В	219	38.667	11.618	-4.422	1.00	21.35

FIGURE 3 (Cont.)CV

A	В	С	D	E		F		G		Н	I	J
7601	С	ALA	В	219	3	9.340	13	.818	_	3.523	1.00	21.64
7602	0	ALA		219		8.756		.587		4.270		20.84
7603	N	LEU		220		9.563		.090		2.240	1.00	
7605	CA	LEU		220		9.003		.285		1.600	1.00	
7607	СВ	LEU		220		9.340		.335		0.110		22.43
7610	CG	LEU		220		8.407		.580		0.840		22.95
7612	CD1	LEU		220		8.991		.642		2.244		24.14
7616	CD2	LEU		220		7.002		.153		0.810		24.62
7620	C	LEU		220		9.364		.616	_	2.239		21.85
7621	ō	LEU		220		8.482		.438		2.393	1.00	
7622	N	PRO		221		0.627		.872		2.583	1.00	
7623	CA	PRO		221		0.969		.150		3.227		22.28
7625	CB	PRO		221		2.442		.987		3.589	1.00	
7628	CG	PRO		221		2.951		.960		2.616	1.00	
7631	CD	PRO		221		1.812		.025		2.379		22.27
7634	C	PRO		221		0.115		.420		4.460		21.79
7635	Ō	PRO		221		9.580		.513		4.592		21.54
7636	N	VAL		222		9.945		.431		5.331		21.34
7638	CA	VAL		222		9.131		.616		6.533		20.96
7640	CB	VAL		222		9.431		.533		7.601	1.00	
7642	CG1	VAL		222		8.492		.664		8.787	1.00	
7646	CG2	VAL		222		0.885		.668		8.085		22.50
7650	C	VAL		222		7.620		.635		6.214		20.48
7651	Ō	VAL		222		6.877		.411		6.804	1.00	
7652	N	LEU		223		7.172		.773		5.307	1.00	
7654	CA	LEU		223		5.750		.717		4.924	1.00	
7656	СВ	LEU		223		5.466		.562		3.957	1.00	
7659	CG	LEU		223		5.293		.173		4.587		21.95
7661	CD1	LEU		223		5.296		.095		3.512		22.04
7665	CD2	LEU		223		4.039		.111		5.407	1.00	
7669	С	LEU		223		5.327		.015		4.253	1.00	
7670	0	LEU		223		4.188		.456		4.381	1.00	
7671	N	ASP	В	224		6.250		.599		3.503	1.00	
7673	CA	ASP		224		6.042	19	.893	_	2.883	1.00	
7675	CB	ASP	В	224		7.272	20	.287		2.069	1.00	
7678	CG	ASP	В	224		7.289	19	.671	_	0.705	1.00	22.67
7679	OD1	ASP	В	224	3	6.256	19	.094	-	0.288	1.00	23.35
7680	OD2	ASP	В	224	3	8.304	19	.744		0.036	1.00	25.14
7681	С	ASP	В	224		5.778	20	.972	-	3.908		19.81
7682	0	ASP	В	224	3	4.910	21	. 795	-	3.702	1.00	19.95
7683	N	LYS	В	225	3	6.541	20	.990	_	4.996	1.00	19.94
7685	CA	LYS	В	225	3	6.368	22	.027	_	6.013	1.00	20.31
7687	CB	LYS	В	225	3	7.525	22	.048	_	7.022	1.00	20.63
7690	CG	LYS	В	225	3	8.973	22	.184	-	6.439	1.00	22.72
7693	CD I	BLYS	В	225	3	9.100	23	.053	-	5.155	0.35	21.46
7694	CD Z	ALYS	В	225	3	9.001	22	.753	-	5.014	0.65	25.09
7699	CE I	BLYS	В	225	3	9.223	22	.270	-	3.837	0.35	19.92
7700		ALYS		225	3	9.871		.974	-	4.801	0.65	25.51
7705		BLYS		225	4	0.570	21	.728	-	3.502	0.35	14.63
7706		ALYS		225		9.377		.575		3.546	0.65	24.29
7713	C	LYS		225		5.049		.804		6.718	1.00	
7714	0	LYS	В	225	3	4.320	22	.762	-	6.982	1.00	19.64

FIGURE 3 (Cont.) CW

Α	В	С	D	E	F	G	Н	I	J
7715	N	TYR	В	226	34.733	20.536	-6.979	1.00	19.10
7717	CA	TYR		226	33.437	20.151	-7.525	1.00	18.47
7719	СВ	TYR		226	33.307	18.624	-7.646	1.00	18.62
7722	CG	TYR		226	31.883	18.168	-7.875	1.00	17.81
7723	CD1	TYR		226	31.300	18.256	-9.132	1.00	17.52
7725	CE1	TYR		226	29.994	17.859	-9.337	1.00	20.05
7727	CZ	TYR		226	29.232	17.374	-8.279	1.00	18.47
7728	ОН	TYR		226	27.919	16.982	-8.500	1.00	17.52
7730	CE2	TYR	В	226	29.785	17.299	-7.026	1.00	17.57
7732	CD2	TYR	В	226	31.112	17.694	-6.829	1.00	17.49
7734	С	TYR	В	226	32.331	20.699	-6.643	1.00	18.41
7735	0	TYR	В	226	31.452	21.411	-7.122	1.00	18.11
7736	N	ALA	В	227	32.417	20.408	-5.345	1.00	18.13
7738	CA	ALA	В	227	31.403	20.799	-4.377	1.00	18.18
7740	CB	ALA	В	227	31.723	20.221	-3.021	1.00	17.94
7744	С	ALA	В	227	31.281	22.316	-4.251	1.00	18.61
7745	0	ALA	В	227	30.196	22.851	-4.063	1.00	18.11
7746	N	GLU	В	228	32.407	22.996	-4.328	1.00	19.06
7748	CA	GLU	В	228	32.418	24.439	-4.177	1.00	20.24
7750	CB	GLU		228	33.864	24.949	-4.123	1.00	20.64
7753	CG	GLU		228	34.451	24.809	-2.730	1.00	23.29
7756	CD	GLU		228	35.947	24.586	-2.731	1.00	26.70
7757		GLU		228	36.464	23.942	-1.768	1.00	29.92
7758	OE2	GLU		228	36.592	25.044	-3.686	1.00	27.85
7759	C	GLU		228	31.636	25.080	-5.300	1.00	20.03
7760	0	GLU		228	30.842	25.982	-5.063	1.00	20.42
7761	N	SER		229	31.824	24.584	-6.521	1.00	20.10
7763	CA	SER		229	31.140	25.146	-7.663	1.00	20.21
7765	CB	SER		229	31.838	24.755	-8.958	1.00	20.74
7768	OG	SER		229	33.134	25.319	-8.986	1.00	21.81
7770	C	SER		229	29.655	24.795	-7.704	1.00	19.69
7771 7 77 2	N O	SER ILE		229	28.845	25.675	-7.972	1.00	19.58
7774	CA	ILE	В	230 230	29.283	23.538	-7.451	1.00	19.26
7776	CB	ILE		230	27.855 27.588	23.173 21.634	-7.467 -7.493	1.00	19.00
7778	CG1		В	230	28.132	20.922	-6.249	1.00	19.39 19.42
7781	CD1	ILE		230	27.348	19.661	-5.883	1.00	19.42
7785	CG2	ILE		230	28.145	20.996	-8.778		20.74
7789	C	ILE		230	27.118	23.798	-6.292	1.00	18.75
7790	Ö	ILE		230	25.934	24.062	-6.404	1.00	
7791	N	GLY		231	27.825	24.000	-5.179	1.00	17.92
7793	CA	GLY		231	27.260	24.588	-3.977	1.00	18.54
7796	С	GLY		231	26.885	26.044	-4.189	1.00	18.41
7797	0	GLY		231	25.776	26.467	-3.838		18.39
7798	N	LEU		232	27.791	26.809	-4.801		18.03
7800	CA	LEU		232	27.463	28.191	-5.176	1.00	17.92
7802	CB	LEU	В	232	28.697	28.973	-5.644	1.00	17.76
7805	CG	LEU	В	232	28.471	30.416	-6.137	1.00	18.58
7807		LEU		232	27.676	31.245	-5.123	1.00	20.10
7811		LEU		232	29.783	31.085	-6.471	1.00	19.77
7815	C	LEU		232	26.371	28.184	-6.232	1.00	17.69
7816	0	LEU	В	232	25.391	28.929	-6.125	1.00	17.69

FIGURE 3 (Cont.)CX

A	В	С	D	E	F	G	Н	I	J
7817	N	ALA	В	233	26.520	27.332	-7.243	1.00	17.54
7819	CA	ALA		233	25.535	27.255	-8.330	1.00	17.52
7821	CB	ALA		233	25.937	26.175	-9.322	1.00	17.72
7825	C	ALA		233	24.133	26.996	-7.801	1.00	16.87
7826	0	ALA		233	23.149	27.503	-8.321	1.00	16.72
7827	N	PHE		234	24.055	26.207	-6.738	1.00	17.20
7829	CA	PHE		234	22.796	25.770	-6.175	1.00	17.20
7831	СВ	PHE		234	23.077	24.798	-5.020	1.00	17.86
7834	CG	PHE		234	21.913	23.952	-4.635	1.00	19.19
7835	CD1	PHE		234	21.908	22.595	-4.939	1.00	
7837	CE1	PHE		234	20.833	21.786	-4.576	1.00	
7839	CZ	PHE		234	19.753	22.346	-3.895	1.00	
7841	CE2	PHE		234	19.766	23.705	-3.578	1.00	
7843	CD2	PHE		234	20.837	24.489	-3.936	1.00	19.81
7845	C		В	234	22.023	26.972	-5.659	1.00	
7846	0		В	234	20.817	27.075	-5.856	1.00	16.09
7847	N	GLN		235	22.724	27.860	-4.969	1.00	16.71
7849	CA	GLN		235	22.093	29.040	-4.427	1.00	17.18
7851	СВ	GLN		235	22.918	29.661	-3.304	1.00	16.88
7854	CG	GLN		235	22.173	30.781	-2.566	1.00	16.78
7857	CD	GLN		235	20.856	30.332	-1.970	1.00	18.18
7858	OE1	GLN		235	20.783	29.271	-1.353	1.00	17.96
7859	NE2	GLN		235	19.818	31.140	-2.138	1.00	15.32
7862	С	GLN		235	21.821	30.089	-5.501	1.00	16.98
7863	0	GLN		235	20.842	30.800	-5.392	1.00	16.15
7864	N	VAL		236	22.640	30.184	-6.544	1.00	17.46
7866	CA	VAL		236	22.265	31.160	-7.590	1.00	18.23
7868	CB	VAL	В	236	23.405	31.708	-8.547	1.00	18.68
7870	CG1	VAL	В	236	24.747	31.119	-8.271	1.00	19.87
7874	CG2	VAL	В	236	23.019	31.733	-10.030	1.00	19.70
7878	С	VAL	В	236	21.003	30.665	-8.279	1.00	17.45
7879	0	VAL	В	236	20.139	31.457	-8.531	1.00	17.04
7880	N	GLN	В	237	20.856	29.350	-8.447	1.00	17.88
7882	CA	GLN	В	237	19.649	28.785	-9.035	1.00	18.28
7884	CB	GLN	В	237	19.783	27.288	-9.337	1.00	18.86
7887	CG	GLN	В	237	18.561	26.715	-10.056	1.00	20.61
7890	CD	GLN		237	18.402	27.211	-11.478	1.00	23.91
7891		GLN		237	19.207		-11.962		27.71
7892	NE2			237	17.361	26.738	-12.157	1.00	25.53
7895	С	GLN		237	18.469	29.005	-8.135	1.00	17.68
7896	0	GLN		237	17.381	29.326	-8.612	1.00	18.18
7897	N	ASP		238	18.673	28.830	-6.832	1.00	16.95
7899	CA	ASP		238	17.624	29.133	-5.872	1.00	16.59
7901	CB	ASP		238	18.084	28.803	-4.452	1.00	
7904	CG	ASP		238	16.988	28.976	-3.451	1.00	
7905	OD1	ASP		238	16.037	28.162	-3.445	1.00	
7906		ASP		238	16.959	29.929	-2.651	1.00	
7907	C	ASP		238	17.186	30.610	-5.985	1.00	
7908	O N	ASP		238	16.001	30.905	-5.932	1.00	
7909 7911	N Ca	ASP ASP		239	18.135	31.526	-6.146	1.00	
7911 7913	CA CB	ASP		239 239	17.799	32.959	-6.321 -6.321	1.00	
1213	CD	ASP	D	437	19.044	33.819	-6.384	1.00	19.28

FIGURE 3 (Cont.)CY

Α	В	С	D	E	F	G	Н	I	J
7916	CG	ASP	В	239	19.766	33.928	-5.070	1.00	19.95
7917		ASP		239	19.251	33.447	-4.018		23.46
7918		ASP		239	20.886	34.480	-5.016	1.00	19.63
7919	C	ASP		239	17.021	33.192	-7.610	1.00	19.87
7920	Ō	ASP		239	16.020	33.917	-7.629	1.00	20.25
7921	N	ILE		240	17.492	32.570	-8.687	1.00	19.96
7923	CA	ILE		240	16.845	32.676	-9.986	1.00	20.61
7925	СВ	ILE		240	17.647	31.902	-11.039	1.00	20.77
7927	CG1	ILE		240	18.945	32.645	-11.363	1.00	
7930	CD1	ILE		240	19.974	31.792	-11.997	1.00	21.71
7934	CG2	ILE		240	16.821	31.682	-12.304	1.00	21.31
7938	C	ILE		240	15.413	32.161	-9.932		
7939	0	ILE		240	14.506	32.784	-10.482	1.00	20.05
7940	N	LEU		241	15.214	31.014	-9.283		21.23
7942	CA	LEU		241	13.904	30.394	-9.206		21.82
7944	СВ	LEU		241	14.009	28.986	-8.620	1.00	22.08
7947	CG	LEU		241	14.569	27.953	-9.600	1.00	
7949	CD1			241	14.635	26.592	-8.926	1.00	
7953	CD2	LEU		241	13.740	27.874	-10.869	1.00	
7957	C	LEU		241	12.955	31.226	-8.384		22.17
7958	Ö	LEU		241	11.759	31.219	-8.613	1.00	22.86
7959	N	ASP		242	13.487	31.928	-7.401	1.00	22.89
7961	CA	ASP		242	12.680	32.816	-6.597	1.00	23.68
7963	СВ	ASP		242	13.538	33.476	-5.526		24.26
7966	CG	ASP		242	12.782	33.732	-4.261		26.59
7967		ASP		242	12.339	34.885	-4.081		29.09
7968		ASP		242	12.586	32.842	-3.395	1.00	30.35
7969	C	ASP		242	12.018	33.889	-7.468	1.00	24.03
7970	ō	ASP		242	10.872	34.264	-7.225		23.75
7971	N	VAL		243	12.722	34.380	-8.478		24.22
7973	CA	VAL		243	12.133	35.431	-9.334		25.09
7975		BVAL		243	13.207	36.455	-9.871	0.35	24.92
7976		AVAL		243	13.180	36.479	-9.849		25.18
7979		BVAL		243	14.454	35.767	-10.368		24.74
7980		AVAL		243	14.270	36.727	-8.817		24.27
7987		BVAL		243	12.633	37.361	-10.975	0.35	23.96
7988		AVAL		243	13.775	36.088	-11.166		25.87
7995	С	VAL		243	11.271	34.851	-10.474		25.74
7996	0	VAL		243	10.167	35.330	-10.688		25.89
7997	N	VAL		244	11.745	33.812	-11.160		26.96
7999	CA	VAL	В	244	11.065	33.282	-12.350		27.89
8001	CB	VAL	В	244	12.069	32.914	-13.472		28.15
8003	CG1	VAL		244	12.996	34.083	-13.769		29.48
8007	CG2	VAL		244	12.852				28.31
8011	C	VAL		244	10.158		-12.136		28.41
8012	0	VAL		244	9.330		-12.983		28.51
8013	N	GLY		245	10.331	31.335			29.07
8015	CA	GLY		245	9.583	30.107	-10.813		29.72
8018	С	GLY		245	8.131	30.378		1.00	
8019	0	GLY		245	7.793	31.482	-10.070	1.00	
8020	N	ASP	В	246	7.276	29.376	-10.613		30.83
8022	CA	ASP	В	246	5.885	29.465	-10.194	1.00	31.66

FIGURE 3 (Cont.)CZ

A	В	С	D	E	F	G	Н	I	J
8024	СВ	ASP	В	246	4.996	28.632	-11.128	1.00	32.32
8027	CG	ASP		246	3.527	29.006	-11.027	1.00	35.80
8028	OD1			246	2.981	29.516	-12.041		41.36
8029			В	246	2.818	28.820	-9.997	1.00	39.19
8030	C	ASP		246	5.782	28.894	-8.790	1.00	30.65
8031	o	ASP		246	6.321	27.842	-8.546	1.00	30.56
8032	N	THR		247	5.072	29.572	-7.892	1.00	29.92
8034	CA	THR		247	4.846	29.080	-6.533	1.00	29.76
8036	CB	THR		247	3.814	29.975	-5.811	1.00	29.76
8038	OG1	THR		247	4.378	31.272	-5.593	1.00	31.54
8040	CG2	THR		247	3.502	29.459	-4.399	1.00	30.40
8044	C	THR		247	4.401	27.611	-6.492	1.00	28.88
8045	0	THR		247	4.911	26.844			28.30
8046	N	ALA		248	3.465	27.222	-5.685 -7.358	1.00	
8048	CA	ALA		248	2.932	25.852			28.23
8050	CB	ALA		248	1.809	25.708	-7.367	1.00	28.33
8054	C	ALA		248	4.007	24.805	-8.391 -7.644	1.00	28.17 28.26
8055	0	ALA		248	3.925	23.687			
8056	N	THR		249	4.985	25.172	-7.143 -9.466	1.00	28.69
8058	CA	THR		249	6.091	24.292	-8.466 -8.824	1.00	27.77
8060	CB	THR		249	6.638	24.726	-10.188		
8062	OG1	THR		249	5.596	24.726	-11.164	1.00	27.90
8064	CG2	THR		249	7.706	23.767	-10.678	1.00	30.21
8068	C	THR		249	7.708	24.275	-7.773	1.00	28.58
8069	0	THR		249					26.85
8070	N	LEU		250	7.671	23.202	-7.356	1.00	26.31
8070	CA	LEU		250	7.654 8.706	25.463 25.627	-7.348	1.00	25.98
8074	CB	LEU		250	8.994	27.116	-6.328 -6.091	1.00	25.67
8077	CG	LEU		250	9.408	28.030		1.00	25.92
8079	CD1	LEU		250	9.656	29.433	-7.239 -6.691	1.00	
8083	CD2	LEU		250	10.625	27.516	-7.954	1.00	27.93 28.70
8087	C	LEU		250	8.359	25.039	-4.965	1.00	24.61
8088	0	LEU		250	9.244	24.625	-4.217	1.00	22.99
8089	N	GLY		251	7.077	25.078	-4.612	1.00	23.96
8091	CA	GLY		251	6.636	24.759	-3.265	1.00	23.66
8094	C	GLY		251	6.808	25.892	-2.263	1.00	23.66
8095	0	GLY		251	6.449	25.748	-1.105	1.00	23.25
8096	N	LYS		252	7.310	27.036	-2.721		23.45
8098	CA	LYS		252	7.499	28.207	-1.881		23.55
8100	CB	LYS		252	8.913	28.217	-1.262		23.19
8103	CG	LYS		252	10.065	28.100	-2.279		22.81
8106	CD	LYS		252	11.443	27.892	-1.587		21.30
8109	CE	LYS		252	12.575	28.125	-2.537		19.95
8112	NZ	LYS		252	13.876	27.549	-2.087		18.06
8116	С	LYS		252	7.248	29.466	-2.729		24.42
8117	0	LYS		252	7.280	29.414	-3.961		24.38
8118	N	ARG		253	7.024	30.592	-2.066		25.44
8120	CA	ARG		253	6.534	31.795	-2.744		26.73
8122	CB	ARG		253	6.006	32.830	-1.737		27.67
8125	CG	ARG		253	4.510	33.101	-1.907		31.24
8128	CD	ARG		253	3.825	33.710	-0.700		35.52
8131	NE	ARG		253	3.150	32.704	0.116		37.39

FIGURE 3 (Cont.)DA

Α	В	С	D	E	F	G	Н	I	J
8133	CZ	ARG	В	253	2.036	32.056	-0.235	1 00	39.88
8134	NH1	ARG		253	1.451	32.263	-1.417	1.00	
8137	NH2	ARG		253	1.518	31.167	0.605	1.00	
8140	С	ARG		253	7.550	32.432	-3.685	1.00	
8141	ō	ARG		253	8.642	32.852	-3.283		25.79
8142	N	GLN		254	7.176	32.480	-4.955	1.00	25.68
8144	CA	GLN		254	7.848	33.323	-5.931		25.41
8146	СВ	GLN		254	7.076	33.337	-7.255		25.85
8149		BGLN		254	7.707	34.187	-8.363		25.46
8150		AGLN		254	7.696	34.266	-8.323		26.52
8155		BGLN		254	7.388	35.665	-8.261	0.35	
8156		AGLN		254	6.858	34.376	-9.595		29.40
8157		BGLN		254	8.227	36.501	-8.593	0.35	
8158		AGLN		254	7.335	34.901	-10.609	0.65	
8159		BGLN		254	6.180	35.993	-7.809		25.98
8160		AGLN		254	5.622	33.888	-9.547	0.65	29.10
8165	C	GLN		254	7.900	34.730	-5.369		24.67
8166	ō	GLN		254	6.942	35.184	-4.755		24.03
8167	N	GLY		255	9.023	35.413	-5.565		24.23
8169	CA	GLY		255	9.107	36.829	-5.264		24.15
8172	C	GLY		255	9.417	37.151	-3.816		24.34
8173	ō	GLY		255	9.464	38.307	-3.465		24.07
8174	N	ALA		256	9.656	36.142	-2.983		24.66
8176	CA	ALA		256	9.909	36.359	-1.559		25.08
8178	CB	ALA		256	9.978	35.024	-0.833		24.93
8182	C	ALA		256	11.179	37.180	-1.288		25.56
8183	ō	ALA		256	11.213	37.979	-0.353	1.00	26.42
8184	N	ASP		257	12.210	37.000	-2.105	1.00	25.88
8186	CA	ASP		257	13.466	37.739	-1.932	1.00	26.25
8188	СВ	ASP		257	14.564	37.191	-2.848		26.11
8191	CG	ASP		257	15.025	35.791	-2.463	1.00	
8192	OD1		В	257	14.815	35.353	-1.299	1.00	26.12
8193	OD2	ASP	В	257	15.602	35.054	-3.292	1.00	
8194	С	ASP		257	13.286	39.221	-2.241		27.05
8195	0	ASP	В	257	13.823	40.074	-1.549	1.00	
8196	N	GLN	В	258	12.545	39.520	-3.304	1.00	28.65
8198	CA	GLN	В	258	12.278	40.908	-3.691	1.00	29.67
8200	CB :	BGLN	В	258	11.590	40.972	-5.061	0.35	29.64
8201	CB .	AGLN	В	258	11.557	40.939	-5.046	0.65	30.10
8206	CG	BGLN	В	258	12.546	40.710	-6.226	0.35	29.64
8207	CG .	AGLN	В	258	11.357	42.333	-5.625	0.65	31.67
8212	CD	BGLN	В	258	11.961	41.060	-7.589	0.35	29.88
8213	CD .	AGLN	В	258	9.896	42.666	-5.883	0.65	33.37
8214	0E1	BGLN	В	258	12.242	40.380	-8.581	0.35	29.18
8215	OE1	AGLN	В	258	9.502	42.893	-7.025	0.65	34.64
8216		BGLN		258	11.163	42.126	-7.646	0.35	29.79
8217	NE2	AGLN	В	258	9.094	42.705	-4.820	0.65	34.91
8222	C	GLN		258	11.455	41.638	-2.614		29.97
8223	0	GLN		258	11.755	42.780	-2.274		29.34
8224	N	GLN		259	10.439	40.957	-2.080		30.70
8226	CA	GLN		259	9.658	41.427	-0.922		31.61
8228	CB	GLN	В	259	8.769	40.285	-0.410	1.00	32.41

FIGURE 3 (Cont.)DB

Α	В	С	D	E	F	G	H	I	J
8231	CG	GLN	В	259	7.466	40.703	0.244	1.00	35.31
8234	CD	GLN		259	6.317	40.769	-0.744	1.00	39.68
8235	OE1	GLN		259	5.925	41.861	-1.174	1.00	43.25
8236	NE2	GLN		259	5.780	39.605	-1.119	1.00	42.40
8239	C	GLN		259	10.546	41.934	0.242	1.00	31.29
8240	Ō	GLN		259	10.321	43.032	0.776	1.00	31.47
8241	N	LEU		260	11.552	41.135	0.612	1.00	30.18
8243	CA	LEU		260	12.421	41.420	1.761	1.00	29.88
8245	CB	LEU		260	12.851	40.109	2.446	1.00	29.79
8248	CG	LEU		260	11.792	39.268	3.160	1.00	30.18
8250	CD1	LEU		260	12.453	38.363	4.192	1.00	29.62
8254	CD2	LEU		260	10.742	40.140	3.817	1.00	31.47
8258	C	LEU		260	13.681	42.207	1.413	1.00	28.94
8259	0	LEU		260	14.431	42.593	2.307	1.00	
8260	N	GLY		261	13.921	42.429	0.128	1.00	27.95
8262	CA	GLY		261	15.133	42.429	-0.333	1.00	
8265	C	GLY		261			-0.333		26.93
8266	0				16.398	42.279		1.00	25.88
8267	N	GLY		261	17.436	42.845	0.261	1.00	25.61
	CA	LYS		262	16.325	40.959	-0.277	1.00	24.82
8269		LYS		262	17.501	40.115	-0.136	1.00	23.75
8271	CB	LYS		262	17.153	38.627	-0.295	1.00	23.56
8274	CG	LYS		262	16.230	38.069	0.762	1.00	23.25
8277	CD			262	16.916	37.862	2.096	1.00	21.56
8280	CE	LYS		262	15.901	37.433	3.158	1.00	23.14
8283	NZ		В	262	16.536	37.070	4.482		21.85
8287	С	LYS		262	18.515	40.497	-1.195	1.00	23.58
8288	0	LYS		262	18.145	40.845	-2.337	1.00	23.29
8289	N	SER		263	19.785	40.474	-0.803	1.00	22.82
8291	CA	SER		263	20.885	40.514	-1.746	1.00	22.51
8293	CB	SER		263	22.206	40.785	-1.035	1.00	22.93
8296	OG	SER		263	22.263	42.141	-0.613	1.00	23.10
8298	C	SER		263	20.934	39.170	-2.452	1.00	22.79
8299	0	SER		263	21.051	38.122	-1.784	1.00	22.61
8300	N	THR		264	20.786	39.194	-3.782	1.00	21.90
8302	CA	THR		264	20.764	37.973	-4.593	1.00	22.01
8304	CB	THR		264	19.304	37.496	-4.909	1.00	22.17
8306	OG1	THR		264	18.667	38.392	-5.827		23.42
8308	CG2	THR		264	18.386	37.525	-3.707		21.68
8312	C	THR		264	21.499	38.175	-5.908		21.99
8313	0	THR		264	21.731	39.306	-6.354		21.16
8314	N	TYR		265	21.841	37.066	-6.553		21.84
8316	CA	TYR		265	22.470	37.134	-7.864		22.04
8318	CB	TYR		265	22.959	35.754	-8.319		21.34
8321	CG	TYR		265	24.340	35.435	-7.803		20.33
8322	CD1	TYR		265	25.430	35.422	-8.654		20.38
8324	CE1	TYR		265	26.686	35.129	-8.197		20.95
8326	CZ	TYR		265	26.877	34.859	-6.866		20.10
8327	OH	TYR		265	28.142	34.576	-6.417	1.00	
8329	CE2	TYR		265	25.818	34.876	-5.989	1.00	
8331	CD2	TYR		265	24.561	35.161	-6.455	1.00	
8333	C	TYR		265	21.588	37.816	-8.933		22.40
8334	0	TYR	Þ	265	22.075	38.711	-9.612	1.00	22.20

FIGURE 3 (Cont.)DC

A	В	С	D	E	F	G	Н	I	J
8335	N	PRO	В	266	20.328	37.413	-9.102	1.00	22.68
8336	CA	PRO	В	266	19.448	38.083	-10.073		23.28
8338	CB	PRO	В	266	18.131	37.309	-9.984		23.44
8341	CG	PRO	В	266	18.438	36.064	-9.253	1.00	23.26
8344	CD	PRO	В	266	19.635	36.319	-8.412		23.08
8347	C	PRO	В	266	19.193	39.550	-9.744	1.00	23.45
8348	0	PRO	В	266	19.084	40.350	-10.668	1.00	23.18
8349	N	ALA	В	267	19.099	39.890	-8.460	1.00	23.47
8351	CA	ALA	В	267	18.821	41.268	-8.062	1.00	23.58
8353	CB	ALA	В	267	18.569	41.386	-6.560	1.00	23.84
8357	С	ALA	В	267	19.962	42.155	-8.483	1.00	23.82
8358	0	ALA	В	267	19.742	43.216	-9.062	1.00	24.38
8359	N	LEU	В	268	21.184	41.692	-8.247	1.00	23.53
8361	CA	LEU	В	268	22.375	42.447	-8.586	1.00	23.59
8363	CB	LEU	В	268	23.566	41.908	-7.798	1.00	23.51
8366	CG	LEU	В	268	24.934	42.511	-8.113	1.00	23.92
8368	CD1	LEU	В	268	24.947	44.021	-7.830	1.00	24.92
8372	CD2	LEU	В	268	26.012	41.800	-7.318	1.00	24.12
8376	C	LEU	В	268	22.704	42.437	-10.082	1.00	23.25
8377	0	LEU	В	268	22.964	43.479	-10.664	1.00	23.31
8378	N	LEU	В	269	22.693	41.253	-10.683	1.00	22.76
8380	CA	LEU	В	269	23.281	41.018	-11.995	1.00	22.56
8382	CB	LEU	В	269	24.093	39.726	-11.983	1.00	22.53
8385	CG	LEU	В	269	25.314	39.686	-11.062	1.00	24.16
8387	CD1	LEU	В	269	25.881	38.277	-11.022	1.00	25.08
8391	CD2	LEU	В	269	26.394	40.674	-11.518	1.00	25.88
8395	С	LEU	В	269	22.237	40.925	-13.089	1.00	21.93
8396	0	LEU	В	269	22.567	40.925	-14.273	1.00	21.98
8397	N	GLY	В	270	20.981	40.880	-12.696	1.00	21.10
8399	CA	GLY		270	19.925	40.537	-13.619	1.00	21.48
8402	C	GLY		270	19.923	39.035	-13.860	1.00	21.79
8403	0	GLY		270	20.883	38.320		1.00	20.41
8404	N	LEU		271	18.831	38.570			22.27
8406	CA	LEU		271	18.587		-14.645		23.11
8408	CB	LEU		271	17.169	36.923			23.57
8411	CG	LEU		271	16.145		-14.051		23.96
8413		LEU		271	14.712		-14.638		25.68
8417		LEU		271	16.375		-13.152		24.82
8421	C	LEU		271	19.554		-15.601		23.62
8422	0	LEU		271	19.999		-15.348		22.96
8423	N	GLU		272	19.885		-16.704		24.28
8425	CA	GLU		272	20.703		-17.715		25.35
8427	CB	GLU		272	20.712		-19.049		26.22
8430	CG	GLU		272	21.247		-20.184		30.72
8433	CD	GLU		272	20.177		-20.858		36.13
8434		GLU		272	19.801		-22.020		40.61
8435 8436	OE2 C	GLU GLU		272	19.725		-20.244		38.13
	0	GLU		272	22.116		-17.220		24.46 23.99
8437 8438	N	GLU		272 273	22.658 22.707		-17.405 -16.582		23.99
8440	CA	GLN		273	24.052		-16.582		23.54
8442	CB	GLN		273	24.052		-15.569		23.89
U774	CD	CHIA	ט	213	24.040	20.400	13.303	1.00	43.73

FIGURE 3 (Cont.)DD

Α	В	С	D	E	F	G	Н	I	J
8445	CG	GLN		273	25.057		-16.701		26.62
8448	CD	GLN		273	25.436	40.804			29.62
8449	OE1	GLN		273	26.041		-15.140	1.00	29.56
8450	NE2	GLN		273	25.046	41.834	-16.941	1.00	32.63
8453	C	GLN		273	24.042	36.157	-14.848	1.00	23.16
8454	0	GLN		273	24.994	35.428	-14.656	1.00	23.94
8455	N	ALA		274	22.968	36.130	-14.071	1.00	22.86
8457	CA	ALA		274	22.852	35.161	-12.985	1.00	22.78
8459	CB	ALA		274	21.591	35.413	-12.169	1.00	22.56
8463	С	ALA		274	22.848	33.738		1.00	22.60
8464	0	ALA		274	23.542	32.873	-13.071	1.00	22.64
8465	N	ARG	В	275	22.085	33.520		1.00	22.89
8467	CA	ARG	В	275	22.048	32.213	-15.299	1.00	23.30
8469	СВ	ARG	В	275	21.012	32.205	-16.431	1.00	23.67
8472	CG	ARG	В	275	19.594	32.090	-15.944	1.00	25.28
8475	CD	ARG	В	275	18.542	32.199	-17.031	1.00	27.92
8478	NE	ARG	В	275	17.209	31.888	-16.503	1.00	30.36
8480	CZ	ARG	В	275	16.104	32.616	-16.697	1.00	32.35
8481	NH1	ARG	В	275	16.121	33.727	-17.423	1.00	31.95
8484	NH2	ARG	В	275	14.954	32.217	-16.160	1.00	34.03
8487	С	ARG	В	275	23.424	31.827	-15.854	1.00	23.20
8488	0	ARG	В	275	23.843	30.669	-15.783	1.00	22.27
8489	N	LYS	В	276	24.111	32.807	-16.421	1.00	23.01
8491	CA	LYS	В	276	25.418	32.595	-16.998	1.00	22.90
8493	CB	LYS	В	276	25.870	33.833	-17.774	1.00	23.16
8496	CG	LYS	В	276	27.307	33.794	-18.251	1.00	24.89
8499	CD	LYS	В	276	27.542	32.619	-19.190	1.00	28.29
8502	CE	LYS	В	276	28.672	32.892	-20.166	1.00	29.58
8505	NZ	LYS	В	276	29.948	33.113	-19.451	1.00	30.99
8509	C	LYS	В	276	26.422	32.253	-15.893	1.00	22.40
8510	0	LYS	В	276	27.270	31.400	-16.086	1.00	22.05
8511	N	LYS	В	277	26.312	32.901	-14.742	1.00	21.92
8513	CA	LYS	В	277	27.191	32.604	-13.612	1.00	22.26
8515	CB	LYS	В	277	26.959	33.566	-12.444	1.00	22.86
8518	CG	LYS	В	277	27.325	35.029	-12.759	1.00	26.57
8521	CD	LYS	В	277	28.574	35.530	-12.019	1.00	30.08
8524	CE	LYS	В	277	29.067	36.885	-12.583	1.00	31.95
8527	NZ	LYS	В	277	30.540	37.060	-12.449	1.00	33.10
8531	C	LYS	В	277	26.982	31.151	-13.175	1.00	21.47
8532	0	LYS	В	277	27.939	30.422	-12.944	1.00	21.43
8533	N	ALA	В	278	25.725	30.729	-13.101	1.00	20.57
8535	CA	ALA	В	278	25.408	29.366	-12.697	1.00	20.64
8537	CB	ALA	В	278	23.881	29.171	-12.552	1.00	20.42
8541	C	ALA	В	278	25.990	28.377	-13.699	1.00	20.27
8542	0	ALA	В	278	26.607	27.383	-13.306	1.00	19.24
8543	N	ARG	В	279	25.819	28.639	-14.990		20.74
8545	CA	ARG	В	279	26.307	27.695	-15.997		21.12
8547	CB	ARG	В	279	25.765	28.003	-17.392	1.00	21.76
8550	CG	ARG	В	279	26.088	26.897	-18.402		22.89
8553	CD	ARG	В	279	25.654	27.222	-19.814	1.00	25.89
8556	NE	ARG	В	279	26.498		-20.382	1.00	26.63
8558	CZ	ARG	В	279	26.296	28.833	-21.562	1.00	26.13

FIGURE 3 (Cont.) DE

8559 NH1 ARG B 279 25.253 28.490 -22.311 1.00 24.20 8565 C ARG B 279 27.138 29.760 -21.981 1.00 21.40 8566 C ARG B 279 28.461 26.590 -16.177 1.00 21.07 8567 N ASP B 280 28.461 28.795 -15.766 1.00 21.40 8571 CB ASP B 280 30.370 31.200 -16.579 1.00 22.54 8575 OD1 ASP B 280 30.370 31.200 -16.579 1.00 22.52 8575 OD1 ASP B 280 30.138 30.759 -17.724 1.00 26.91 8576 OD2 ASP B 280 30.430 27.952 -17.724 1.00 20.06 8576 OD2 ASP B 280 <t< th=""><th>A</th><th>В</th><th>С</th><th>D</th><th>E</th><th>F</th><th>G</th><th>Н</th><th>I</th><th>J</th></t<>	A	В	С	D	E	F	G	Н	I	J
8562 NH2 ARG B 279 27.138 29.760 -21.981 1.00 21.30 8566 C ARG B 279 27.831 27.650 -16.001 1.00 21.30 8566 N ASP B 280 28.461 28.595 -15.766 1.00 21.40 8567 CA ASP B 280 28.374 -15.595 1.00 21.87 8571 CB ASP B 280 30.375 31.200 -16.579 1.00 25.24 8575 OD1 ASP B 280 30.630 32.424 -16.457 1.00 26.95 8576 OD2 ASP B 280 30.138 30.759 -17.724 1.00 26.91 8577 C ASP B 280 31.440 27.959 -14.456 1.00 26.76 8578 D LEU B 281 29.633 2	8559	NH1	ARG	B	279	25 253	28 490	-22 311	1 00	24 20
8565 C ARG B 279 27.831 27.650 -16.001 1.00 21.07 8567 N ASP B 280 28.461 28.559 -16.177 1.00 21.07 8569 CA ASP B 280 29.915 28.874 -15.595 1.00 21.87 8571 CG ASP B 280 30.335 31.200 -16.579 1.00 22.54 8575 OD1 ASP B 280 30.630 31.200 -16.579 1.00 22.54 8575 OD2 ASP B 280 30.431 27.952 -14.456 1.00 20.76 8576 OD2 ASP B 280 30.414 27.957 -14.562 1.00 20.76 8577 C ASP B 280 31.440 27.97 -14.562 1.00 20.76 8581 CA LEU B 281 2										
8566 O ARG B 279 28.416 26.590 -16.177 1.00 21.07 8567 N ASP B 280 28.461 28.795 -15.766 1.00 21.40 8575 CB ASP B 280 30.335 30.327 -15.313 1.00 22.54 8575 OD1 ASP B 280 30.630 32.424 -16.579 1.00 22.54 8576 OD2 ASP B 280 30.138 30.759 -17.724 1.00 26.91 8577 C ASP B 280 30.401 27.297 -14.562 1.00 20.76 8578 O ASP B 280 31.440 27.297 -14.562 1.00 20.76 8578 O LEU B 281 29.633 27.922 -13.372 1.00 20.76 8578 D LEU B 281 29.633 27.927 -14.562 1.00 19.63 8583 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>										
8567 N ASP B 280 28.461 28.795 -15.766 1.00 21.40 8569 CA ASP B 280 29.915 28.874 -15.513 1.00 22.54 8574 CB ASP B 280 30.337 31.200 -16.579 1.00 25.24 8575 ODL ASP B 280 30.630 32.424 -16.457 1.00 26.91 8576 ODL ASP B 280 30.138 30.7592 -14.456 1.00 21.04 8578 O ASP B 280 31.440 27.297 -14.562 1.00 20.76 8579 N LEU B 281 29.994 27.151 -12.188 1.00 19.69 8581 CA LEU B 281 29.9141 27.569 -10.992 1.00 19.63 8586 CD1 LEU B 281 30.671 24.889 -2.9589 1.00 19.63 8596										
8569 CA ASP B 280 29.915 28.874 -15.595 1.00 21.87 8571 CG ASP B 280 30.370 31.200 -16.579 1.00 22.54 8575 OD1 ASP B 280 30.630 32.424 -16.457 1.00 22.56 8576 OD2 ASP B 280 30.401 27.958 -14.456 1.00 21.04 8577 C ASP B 280 31.440 27.297 -14.556 1.00 20.76 8578 O ASP B 280 31.440 27.297 -14.566 1.00 20.76 8581 CA LEU B 281 29.943 27.151 -12.188 1.00 19.69 8583 CB LEU B 281 29.530 28.953 -10.452 1.00 19.63 8586 CD1 LEU B 281 29.530 29.953 -9.5846 1.00 19.92 8586										
8571 CB ASP B 280 30.335 30.327 -15.313 1.00 22.54 8575 OD1 ASP B 280 30.370 31.200 -16.579 1.00 25.24 8576 OD2 ASP B 280 30.138 30.759 -17.724 1.00 26.91 8577 C ASP B 280 30.401 27.958 -14.456 1.00 20.76 8578 O ASP B 280 31.440 27.297 -14.562 1.00 20.76 8579 N LEU B 281 29.944 27.151 -12.188 1.00 19.69 8581 CB LEU B 281 29.944 27.151 -12.188 1.00 19.69 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 19.69 8586 CG LEU B 281 30.612 28.869 -9.646 1.00 19.99 8596										
8574 CG ASP B 280 30.370 31.200 -16.579 1.00 25.24 8575 OD1 ASP B 280 30.630 32.424 -16.457 1.00 28.05 8577 C ASP B 280 30.401 27.958 -14.456 1.00 21.04 8578 O ASP B 280 31.440 27.297 -14.562 1.00 20.76 8579 N LEU B 281 29.933 27.922 -13.372 1.00 20.21 8581 CA LEU B 281 29.941 27.569 -10.992 1.00 19.69 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 19.63 8586 CD LEU B 281 28.842 29.530 28.953 -10.452 1.00 19.63 8586 CDLEU B 281 28.838 29.532 -9.546 1.00 19.73 8596										
8575 OD1 ASP B 280 30.630 32.424 -16.457 1.00 28.05 8576 C ASP B 280 30.138 30.759 -17.724 1.00 26.91 8578 C ASP B 280 30.401 27.9297 -14.562 1.00 20.76 8579 N LEU B 281 29.633 27.922 -13.372 1.00 20.21 8581 CA LEU B 281 29.934 27.569 -10.992 1.00 19.63 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 19.63 8586 CD LEU B 281 29.838 25.670 -12.468 1.00 19.99 8596 C LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.										
8576 OD2 ASP B 280 30.138 30.759 -17.724 1.00 26.91 8577 C ASP B 280 30.401 27.958 -14.456 1.00 21.04 8578 N LEU B 281 29.633 27.922 -13.372 1.00 20.76 8581 CA LEU B 281 29.994 27.151 -12.188 1.00 19.82 8586 CG LEU B 281 29.9141 27.569 -10.992 1.00 19.82 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 19.63 8598 CD1 LEU B 281 30.812 28.869 -9.646 1.00 19.73 8596 C LEU B 281 30.671 24.889 -12.094 1.00 20.33 8607 CD1 ILE B 282 28.577 23.906 -13.555 1.00 21.14 8602										
8577 C ASP B 280 30.401 27.958 -14.456 1.00 21.04 8578 N ASP B 280 31.440 27.297 -14.562 1.00 20.21 8581 CA LEU B 281 29.934 27.151 -12.188 1.00 19.69 8583 CB LEU B 281 29.944 27.569 -10.992 1.00 19.69 8586 CG LEU B 281 29.530 28.953 -9.646 1.00 19.63 8592 CD2 LEU B 281 29.838 25.670 -12.468 1.00 19.73 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 21.14 8602 CB ILE B 282 28.774 25.295 -13.150 1.00 21.56 8607 <t< td=""><td></td><td>OD2</td><td></td><td>В</td><td></td><td></td><td></td><td></td><td></td><td></td></t<>		OD2		В						
8578 O ASP B 280 31.440 27.297 -14.562 1.00 20.76 8579 N LEU B 281 29.633 27.922 -13.372 1.00 20.76 8581 CA LEU B 281 29.994 27.151 -12.188 1.00 19.69 8586 CB LEU B 281 29.530 28.953 -10.452 1.00 18.53 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 19.63 8592 CD2 LEU B 281 30.812 28.869 -9.646 1.00 19.99 8596 C LEU B 281 30.671 24.889 -12.094 1.00 20.05 8597 O LEU B 282 28.774 25.295 -13.555 1.00 20.35 8597 O LEU B 282 28.597 23.906 -13.555 1.00 21.14 8602 <td< td=""><td>8577</td><td>С</td><td>ASP</td><td>В</td><td></td><td></td><td></td><td></td><td></td><td></td></td<>	8577	С	ASP	В						
8579 N LEU B 281 29.633 27.922 -13.372 1.00 20.21 8581 CA LEU B 281 29.994 27.151 -12.188 1.00 19.69 8583 CB LEU B 281 29.141 27.569 -10.992 1.00 19.63 8586 CG LEU B 281 29.530 28.953 -9.589 1.00 19.63 8592 CD2 LEU B 281 30.812 28.869 -9.546 1.00 19.73 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8600 CB ILE B 282 28.577 23.905 -12.949 1.00 22.56 8604 CG1 ILE B 282 27.190 23.672 -14.076 1.00 22.56 8604 <	8578	0	ASP	В		31.440	27.297	-14.562		
8581 CA LEU B 281 29.994 27.151 -12.188 1.00 19.69 8583 CB LEU B 281 29.141 27.569 -10.992 1.00 19.82 8586 CG LEU B 281 29.530 28.953 -10.452 1.00 18.53 8588 CD1 LEU B 281 28.669 -9.646 1.00 19.99 8596 C LEU B 281 29.838 25.670 -12.468 1.00 19.73 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.555 1.00 21.14 8600 CA ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.672 -14.076 1.00 21.02 8601 CD1 <td< td=""><td>8579</td><td>N</td><td>LEU</td><td>В</td><td>281</td><td></td><td></td><td></td><td>1.00</td><td></td></td<>	8579	N	LEU	В	281				1.00	
8586 CG LEU B 281 29.530 28.953 -10.452 1.00 18.53 8588 CD1 LEU B 281 28.423 29.532 -9.589 1.00 19.63 8596 C LEU B 281 30.812 28.869 -9.646 1.00 19.99 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8602 CB ILE B 282 28.774 25.295 -13.150 1.00 20.33 8604 CG1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8610 C ILE B 282 29.	8581	CA	LEU	В	281	29.994	27.151			
8588 CD1 LEU B 281 28.423 29.532 -9.589 1.00 19.63 8592 CD2 LEU B 281 30.812 28.869 -9.646 1.00 19.99 8596 C LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8600 CA ILE B 282 28.597 23.906 -13.555 1.00 21.14 8602 CB ILE B 282 27.190 23.672 -14.076 1.00 21.02 8607 CDI ILE B 282 26.532 23.265 -12.949 1.00 22.71 8611 CG2 ILE B 282 29.659 23.477 -14.566 1.00 21.32 8615 C ILE B 282 2	8583	СВ	LEU	В	281	29.141	27.569	-10.992	1.00	19.82
8592 CD2 LEU B 281 30.812 28.869 -9.646 1.00 19.99 8596 C LEU B 281 29.838 25.670 -12.468 1.00 19.73 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.03 8598 N ILE B 282 28.774 25.295 -13.150 1.00 21.14 8600 CA ILE B 282 26.178 23.906 -13.555 1.00 21.02 8604 CG1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.62 8615 O ILE B 282 29.659 23.477 -14.566 1.00 21.87 8616 <	8586	CG	LEU	В	281	29.530	28.953	-10.452	1.00	18.53
8596 C LEU B 281 29.838 25.670 -12.468 1.00 19.73 8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8600 CA ILE B 282 28.597 23.906 -13.555 1.00 21.02 8604 CGI ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CDI ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283<	8588	CD1	LEU	В	281	28.423	29.532	-9.589	1.00	19.63
8597 O LEU B 281 30.671 24.889 -12.094 1.00 20.05 8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8600 CA ILE B 282 28.597 23.906 -13.555 1.00 21.14 8602 CB ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CDI ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 26.532 23.477 -14.566 1.00 21.32 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.87 8619 CA ASP B 283 31.12 24.056 -16.430 1.00 22.32 8619 CA	8592	CD2	LEU	В	281	30.812	28.869	-9.646	1.00	19.99
8598 N ILE B 282 28.774 25.295 -13.150 1.00 20.33 8600 CA ILE B 282 28.597 23.906 -13.555 1.00 21.14 8602 CB ILE B 282 27.190 23.672 -14.076 1.00 21.02 8607 CD1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 27.041 22.244 -14.566 1.00 21.32 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 29.659 23.477 -14.488 1.00 21.87 8619 CA ASP B 283 30.132 24.358 -15.487 1.00 21.87 8619	8596	С	LEU	В	281	29.838	25.670	-12.468	1.00	19.73
8600 CA ILE B 282 28.597 23.906 -13.555 1.00 21.14 8602 CB ILE B 282 27.190 23.672 -14.076 1.00 21.02 8604 CG1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 29.659 23.477 -14.664 1.00 21.32 8615 C ILE B 282 29.659 23.477 -14.666 1.00 21.32 8616 O ILE B 282 29.659 23.477 -14.468 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.23 8621 CB ASP B 283 30.410 25.501 -17.330 1.00 22.56	8597	0	LEU	В	281	30.671	24.889	-12.094	1.00	20.05
8602 CB ILE B 282 27.190 23.672 -14.076 1.00 21.02 8604 CG1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 29.659 23.477 -14.564 1.00 21.32 8615 C ILE B 282 29.659 23.477 -14.568 1.00 21.32 8616 O ILE B 282 29.659 23.477 -14.568 1.00 21.32 8617 N ASP B 283 30.149 22.359 -14.488 1.00 21.87 8619 CA ASP B 283 30.032 24.358 -15.487 1.00 21.87 8621 CB ASP B 283 31.412 24.056 -16.430 1.00 22.32 8624	8598	N	ILE	В		28.774	25.295	-13.150	1.00	20.33
8604 CG1 ILE B 282 26.178 23.925 -12.949 1.00 22.56 8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 27.041 22.244 -14.624 1.00 21.66 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 22.32 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.37 8625 OD1 ASP B 283 30.440 25.503 -18.417 1.00 22.23 8625 OD1 ASP B 283 32.369 23.705 -15.624 1.00 22.	8600	CA	ILE	В	282	28.597	23.906	-13.555	1.00	21.14
8607 CD1 ILE B 282 26.532 23.265 -11.610 1.00 22.71 8611 CG2 ILE B 282 27.041 22.244 -14.624 1.00 21.66 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 25.503 -18.417 1.00 22.23 8626 OD2 ASP B 283 30.445 26.623 -18.989 1.00 22.23 8627		CB	ILE	В	282	27.190	23.672	-14.076	1.00	21.02
8611 CG2 ILE B 282 27.041 22.244 -14.624 1.00 21.66 8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.60 8624 CG ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 26.623 -18.989 1.00 26.27 8626 OD2 ASP B 283 32.369 23.705 -15.624 1.00 22.23 8628 O ASP B 283 33.066 22.756 -15.928 1.00 21.47<	8604	CG1		В	282	26.178	23.925	-12.949	1.00	22.56
8615 C ILE B 282 29.659 23.477 -14.566 1.00 21.32 8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.60 8624 CG ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 26.623 -18.989 1.00 26.27 8626 OD2 ASP B 283 32.369 23.705 -15.624 1.00 22.25 8628 O ASP B 283 33.066 22.756 -15.928 1.00 21.47 8629	8607					26.532	23.265		1.00	22.71
8616 O ILE B 282 30.149 22.359 -14.488 1.00 21.92 8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.60 8624 CG ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 26.623 -18.989 1.00 26.27 8626 OD2 ASP B 283 32.369 23.705 -15.624 1.00 22.25 8628 O ASP B 283 33.066 22.756 -15.928 1.00 21.47 8629 N ASP B 284 32.636 24.490 -14.588 1.00 22.34 8631 CA ASP B 284 33.793 24.291 -13.731 1.00 23.34 </td <td></td> <td></td> <td></td> <td>В</td> <td></td> <td>27.041</td> <td>22.244</td> <td>-14.624</td> <td>1.00</td> <td>21.66</td>				В		27.041	22.244	-14.624	1.00	21.66
8617 N ASP B 283 30.032 24.358 -15.487 1.00 21.87 8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.60 8624 CG ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 26.623 -18.989 1.00 26.27 8626 OD2 ASP B 283 29.548 24.676 -18.786 1.00 22.23 8627 C ASP B 283 32.369 23.705 -15.624 1.00 22.25 8628 O ASP B 283 33.066 22.756 -15.928 1.00 21.47 8629 N ASP B 284 32.636 24.490 -14.588 1.00 22.34 8631 CA ASP B 284 33.793 24.291 -13.731 1.00 23.34 8636 CG ASP B 284 35.161 25.368 -11.918 1.				В		29.659	23.477	-14.566		21.32
8619 CA ASP B 283 31.112 24.056 -16.430 1.00 22.32 8621 CB ASP B 283 31.436 25.261 -17.330 1.00 22.60 8624 CG ASP B 283 30.410 25.503 -18.417 1.00 23.70 8625 OD1 ASP B 283 30.445 26.623 -18.989 1.00 26.27 8626 OD2 ASP B 283 29.548 24.676 -18.786 1.00 22.23 8627 C ASP B 283 32.369 23.705 -15.624 1.00 22.25 8628 O ASP B 283 33.066 22.756 -15.928 1.00 21.47 8629 N ASP B 284 32.636 24.490 -14.588 1.00 22.34 8631 CA ASP B 284 33.793 24.291 -13.731 1.00 23.34 8636 CG ASP B 284 35.161 25.569 -12.820 1.00 22.34<										21.92
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		CA								
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FIGURE 3 (Cont.)DF

Α	В	С	D	E	F	G	H	I	J
8658	CG	ARG	В	286	30.138	19 170	-16.097	1.00	28.32
8661		BARG		286	29.468	18.992	-17.466	0.35	
8662		AARG		286	29.453		-17.451	0.65	
8667		BARG		286	29.262		-18.163	0.35	
8668		AARG		286	28.271		-17.365	0.65	
8671		BARG		286	28.839	20.386		0.35	
8672		AARG		286	28.231	16.856	-17.684	0.65	
8673		BARG		286	28.567	19.313	-20.165	0.35	
8674			В	286	29.309	16.209		0.65	
8679			В	286	28.688	21.596	-19.951	0.35	
8680		AARG	В	286	27.089	16.195	-17.563	0.65	
8685	C	ARG		286	33.894	19.108	-15.170	1.00	
8686	ō	ARG		286	34.349	17.988	-15.388		24.81
8687	N	GLN		287	34.651		-15.171	1.00	
8689	CA	GLN		287	36.100		-15.322	1.00	
8691	CB	GLN		287	36.756	21.497		1.00	
8694	CG	GLN		287	36.425	22.206		1.00	
8697	CD	GLN		287	37.009	21.533	-18.012	1.00	
8698				287	38.047	20.880	-17.945	1.00	
8699	NE2	GLN		287	36.340	21.706		1.00	
8702	С	GLN	В	287	36.706	19.364		1.00	
8703	0	GLN		287	37.565	18.521	-14.333	1.00	
8704	N	SER		288	36.241	19.658	-12.905	1.00	
8706	CA	SER	В	288	36.665	18.911	-11.720	1.00	
8708	CB	SER	В	288	36.105	19.510	-10.414	1.00	25.38
8711	OG	SER	В	288	36.557	20.834	-10.215	1.00	24.82
8713	С	SER	В	288	36.289	17.433	-11.820	1.00	25.78
8714	0	SER	В	288	37.077	16.569	-11.459	1.00	25.49
8715	N	LEU	В	289	35.098	17.125	-12.321	1.00	26.38
8717	CA	LEU		289	34.709	15.726	-12.441	1.00	27.10
8719	CB	LEU		289	33.237	15.580	-12.838	1.00	
8722	CG	LEU		289	32.258	15.977	-11.729	1.00	
8724	CD1	LEU		289	30.821	15.804	-12.200	1.00	
8728	CD2	LEU		289	32.524		-10.431	1.00	
8732	C	LEU		289	35.635	14.995	-13.425	1.00	
8733	0	LEU		289	35.998		-13.186	1.00	
8734	N	LYS		290	36.053		-14.487	1.00	
8736	CA CB	LYS LYS		290	36.961		-15.481		30.79
8738 8741	CG	LYS		290 290	37.313 36.966		-16.587 -18.011		30.97 33.97
8744	CD	LYS		290	36.614		-18.921		36.64
8747	CE	LYS		290	35.099		-10.321		37.79
8750	NZ	LYS		290	34.637		-19.343		38.84
8754	C	LYS		290	38.244		-14.809		31.28
8755	Ö	LYS		290	38.750		-15.141		31.44
8756	N	GLN		291	38.759		-13.869		32.13
8758	CA	GLN		291	39.978		-13.152		33.58
8760	СВ	GLN		291	40.470		-12.326	1.00	
8763	CG	GLN		291	40.818		-13.167		35.12
8766	CD	GLN		291	40.846	18.775	-12.353		36.83
8767	OE1	${\tt GLN}$	В	291	41.175		-11.168	1.00	36.95
8768	NE2	GLN	В	291	40.495	19.893	-12.985	1.00	38.40

FIGURE 3 (Cont.)DG

Α	В	С	D	E	٠	F	G	Н	I	J
8771	С	GLN	В	291		39.800	13.810	-12.265	1.00	34.42
8772	ō	GLN		291		40.764	13.098	-12.013		34.62
8773	N	LEU		292		38.577		-11.784	1.00	35.42
8775	CA	LEU		292		38.248		-10.999	1.00	36.35
8777	СВ	LEU		292		36.931	12.542	-10.251	1.00	36.39
8780	CG	LEU		292		36.924	13.515	-9.082	1.00	36.49
8782	CD1	LEU		292		35.562	13.491	-8.411	1.00	36.85
8786	CD2	LEU		292		38.023	13.153	-8.101	1.00	36.84
8790	C	LEU		292		38.141	11.088	-11.820	1.00	37.54
8791	0	LEU		292		38.519	10.015	-11.352	1.00	37.33
8792	N	ALA		293		37.598	11.193	-13.028	1.00	38.95
8794	CA	ALA		293		37.635	10.088	-13.974	1.00	40.14
8796	СВ	ALA		293		36.587	10.291	-15.078	1.00	40.36
8800	C	ALA		293		39.045		-14.565		40.76
8801	0	ALA		293		39.206	9.462			41.94
8802	N	GLU		294		40.045	10.442			41.22
8804	CA	GLU	В	294		41.456	10.118	-14.039		41.53
8806	СВ	GLU		294		42.240	11.402	-14.318	1.00	
8809	CG	GLU		294		43.620	11.186	-14.911	1.00	
8812	CD	GLU		294		44.144	12.428	-15.604		45.96
8813	OE1	GLU		294		44.166	13.499			48.06
8814	OE2	GLU		294		44.528	12.332	-16.794	1.00	47.73
8815	C	GLU		294		42.047	9.414	-12.808		40.89
8816	0	GLU		294		43.185	8.941	-12.846		41.57
8817	N	GLN		295		41.295	9.399	-11.705	1.00	39.90
8819	CA	GLN		295		41.549	8.516		1.00	38.66
8821	СВ	GLN		295		41.248	9.243	-9.243	1.00	38.65
8824	CG	GLN		295		41.958	10.592	-9.083	1.00	38.47
8827	CD	GLN		295		41.556	11.354	-7.816	1.00	37.66
8828	OE1	GLN		295		41.179	10.751	-6.807	1.00	36.11
8829	NE2	GLN	В	295		41.658	12.686	-7.867	1.00	36.75
8832	C	GLN		295		40.681	7.258	-10.689	1.00	37.75
8833	0	GLN		295		40.432	6.560	-9.698	1.00	37.50
8834	N	SER	В	296		40.220	6.995	-11.914	1.00	36.44
8836	CA	SER		296		39.373	5.852		1.00	35.92
8838	CB	SER		296		40.117		-12.022	1.00	36.22
8841	OG	SER		296		39.666		-12.955	1.00	38.05
8843	С	SER		296		38.003	5.810	-11.566		34.56
8844	0	SER		296		37.551	4.753			34.47
8845	N	LEU		297		37.330	6.952			32.72
8847	CA	LEU		297		36.060	7.022			31.10
8849	CB	LEU	В	297		36.114	8.107	-9.699		30.86
8852	CG	LEU	В	297		37.166	7.891	-8.611		30.39
8854	CD1	LEU	В	297		37.381	9.150	-7.786	1.00	30.04
8858	CD2	LEU	В	297		36.771	6.739	-7.721	1.00	30.69
8862	С	LEU	В	297		34.910	7.286	-11.724		30.21
8863	0	LEU	В	297		35.045		-12.684		29.81
8864	N	ASP	В	298		33.776	6.655	-11.425	1.00	28.91
8866	CA	ASP	В	298		32.541	6.834	-12.171	1.00	28.55
8868	CB	ASP		298		31.659	5.597		1.00	28.67
8871	CG	ASP		298		30.377	5.661	-12.823		30.58
8872	OD1	ASP	В	298		30.141	6.682	-13.512	1.00	31.79

FIGURE 3 (Cont.) DH

A	В	С	D	E	F	G	Н	I	J
8873	OD2	ASP	В	298	29.53	4 729	-12.815	1.00	33.35
8874	C	ASP		298	31.83			1.00	27.64
8875	0	ASP		298	31.13			1.00	26.94
8876	N	THR		299	32.00			1.00	26.96
8878	CA	THR		299	31.42		-12.020	1.00	26.33
8880	CB	THR	В	299	32.35		-12.471	1.00	26.05
8882	OG1	THR	В	299	32.57		-13.882	1.00	27.18
8884	CG2	THR	В	299	33.74	0 11.457	-11.879	1.00	26.15
8888	С	THR	В	299	30.00	6 10.704	-12.588	1.00	25.98
8889	0	THR	В	299	29.46	11.785	-12.453	1.00	25.98
8890	N	SER	В	300	29.39	9.682	-13.176	1.00	25.39
8892	CA	SER	В	300	28.13	9.855	-13.906	1.00	25.11
8894	CB	SER	В	300	27.67	2 8.535	-14.531	1.00	25.29
8897	OG	SER	В	300	27.34	6 7.581	-13.529	1.00	27.52
8899	С	SER		300	27.00	10.479	-13.077	1.00	24.18
8900	0	SER		300	26.34			1.00	23.89
8901	N	ALA		301	26.78			1.00	23.33
8903	CA	ALA		301	25.75			1.00	22.98
8905	CB	ALA		301	25.55			1.00	22.98
8909	C	ALA		301	26.05			1.00	22.43
8910	0	ALA		301	25.13			1.00	21.51
8911	N	LEU		302	27.32			1.00	22.10
8913	CA	LEU		302	27.70			1.00	21.91
8915	CB	LEU		302	29.10			1.00	21.74
8918	CG	LEU		302	29.29			1.00	22.89
8920		LEU		302	30.73			1.00	
8924 8928	CD2 C	LEU LEU		302 302	28.33			1.00	23.02
8929	0	LEU		302	27.65 27.41			1.00	22.32
8930	N	GLU		303	27.41			1.00 1.00	21.59 22.83
8932	CA	GLU		303	27.71			1.00	23.58
8934	CB	GLU		303	28.22			1.00	24.19
8937	CG	GLU		303	29.70			1.00	27.75
8940	CD	GLU		303	30.02		-15.962	1.00	31.36
8941	OE1	GLU		303	29.51		-17.070	1.00	34.68
8942	OE2	GLU		303	30.75			1.00	33.57
8943	С	GLU		303	26.24		-13.705		23.21
8944	0	GLU	В	303	25.89	7 16.382	-14.000	1.00	23.30
8945	N	ALA	В	304	25.37		-13.592		22.93
8947	CA	ALA	В	304	23.95	4 14.418	-13.865		23.17
8949	CB	ALA	В	304	23.21	.9 13.063	-13.846	1.00	23.72
8953	С	ALA	В	304	23.34	8 15.383	-12.844	1.00	22.99
8954	0	ALA	В	304	22.53	0 16.240	-13.186	1.00	22.84
8955	N	LEU	В	305	23.78	15.250	-11.596	1.00	22.47
8957	CA	LEU		305	23.33	16.111	-10.518		22.39
8959	CB	LEU		305	23.84	1 15.623			22.42
8962	CG	LEU		305	23.31				23.49
8964		LEU		305	21.81				26.09
8968	CD2	LEU		305	23.83				25.91
8972	C	LEU		305	23.76		-10.732		21.68
8973	O N	LEU		305	22.99		-10.511		21.68
8974	N	ALA	Þ	306	25.00	12 11.142	-11.173	1.00	21.62

FIGURE 3 (Cont.)DI

Α	В	С	D	E	F	•	G	H	I	J
8976	CA	ALA		306		507		-11.401		
8978	CB	ALA		306		970	19.055	-11.829		20.99
8982	С	ALA		306		649	19.827	-12.437		
8983	0	ALA		306		260	20.978	-12.221		20.84
8984	N		В	307		356	19.157	-13.557		
8986	CA	ASP		307		462	19.700	-14.575		
8988	CB	ASP	В	307		298	18.717	-15.749		22.19
8991	CG	ASP	В	307		484	18.721	-16.695		
8992	OD1	ASP	В	307		217	19.734	-16.774		27.76
8993	OD2		В	307		754	17.744	-17.418		28.49
8994	C	ASP		307		091		-13.985		21.17
8995	0	ASP		307		517		-14.199		
8996	N	TYR		308		566	19.037	-13.226		
8998	CA	TYR		308		230	19.196	-12.667		
9000	CB	TYR		308		804	17.946	-11.921		
9003	CG	TYR		308		419	18.039	-11.344		21.19
9004	CD1	TYR		308		220	18.052	-9.966		20.91
9006	CE1	TYR		308		956	18.127	-9.432		21.89
9008	CZ	TYR		308		853	18.187	-10.268		
9009	OH	TYR		308		587	18.254	-9.704		
9011	CE2	TYR		308		020	18.192	-11.643		23.04
9013	CD2	TYR		308		299	18.112	-12.174		22.71
9015	C	TYR		308		145	20.397	-11.726		21.05
9016	O N	TYR		308		109	21.018	-11.613		
9017	N	ILE		309		239	20.713	-11.043		
9019	CA	ILE	В	309		245	21.825	-10.102		21.51
9021 9023	CB CG1	ILE	B B	309 309		635	21.881	-9.382		21.42
9023	CD1			309		663 007	20.817	-8.279		21.51
9030	CG2	ILE		309		891	23.256	-7.593 -8.766		
9034	C			309		874	23.256	-10.774		
9035	0	ILE		309		237	24.017	-10.774		21.41
9036	N	ILE		310		245	23.328	-12.041		22.74
9038	CA	ILE		310		886	24.542	-12.765		23.55
9040	СВ	ILE		310		148	25.209	-13.364		23.89
9042	CG1			310		714	24.400	-14.540		24.25
9045	CD1	ILE		310		776	25.141	-15.342		24.35
9049	CG2	ILE		310		190		-12.269		24.66
9053	C	ILE		310		799	24.344			23.85
9054	ō	ILE		310		400		-14.470		24.70
9055	N	GLN		311		319		-14.015		23.74
9057	CA	GLN		311		251	22.833	-14.990		
9059	CB	GLN		311		584	21.602	-15.821		
9062	CG	GLN		311		713	21.884	-16.815		
9065	CD	GLN		311		172	20.670	-17.588		28.31
9066	OE1	GLN		311		115	20.760	-18.367		
9067	NE2	GLN		311		520	19.540	-17.382		
9070	C	GLN		311		887	22.687	-14.329		
9071	0	GLN	В	311	15.	857	22.873	-14.981		23.30
9072	N	ARG	В	312		889		-13.033		23.14
9074	CA	ARG		312		666		-12.249		22.83
9076	CB	ARG	В	312	16.	010	21.784	-10.806	1.00	22.67

FIGURE 3 (Cont.)DJ

A	В	С	D	E	F	G	Н	I	J
9079	CG	ARG	В	312	16.722	22.887	-10.002	1.00	21.91
9082	CD	ARG		312	17.584	22.348	-8.871		20.80
9085	NE	ARG		312	18.319	23.405	-8.180	1.00	
9087	CZ	ARG		312	17.807	24.145	-7.212		19.88
9088	NH1	ARG	В	312	18.559	25.083	-6.640	1.00	
9091	NH2	ARG	В	312	16.547	23.956	-6.806	1.00	
9094	С	ARG	В	312	14.826	23.434	-12.199	1.00	
9095	0	ARG	В	312	15.361	24.542	-12.222	1.00	
9096	N	ASN	В	313	13.513	23.232	-12.116	1.00	24.23
9098	CA	ASN	В	313	12.519	24.294	-11.967	1.00	25.30
9100	CB	ASN	В	313	11.404	24.132	-13.023	1.00	25.73
9103	CG	ASN	В	313	10.586	22.855	-12.843	1.00	27.06
9104	OD1	ASN	В	313	10.893	22.015	-12.003	1.00	30.28
9105	ND2	ASN	В	313	9.526	22.712	-13.642	1.00	30.33
9108	C	ASN	В	313	11.922	24.303	-10.550	1.00	26.15
9109	0		В	313	10.931	24.991	-10.282	1.00	26.07
9110	N	LYS	В	314	12.523	23.510	-9.663	1.00	26.76
9112	CA	LYS	В	314	12.057	23.349	-8.295	1.00	27.55
9114	CB	LYS	В	314	10.997	22.245	-8.214	1.00	28.24
9117	CG		В	314	11.437	20.876	-8.748	1.00	30.42
9120	CD		В	314	10.388	19.777	-8.483	1.00	34.02
9123	CE		В	314	9.281	19.733	-9.557	1.00	35.81
9126	NZ		В	314	9.763	19.297	-10.914	1.00	37.55
9130	С		В	314	13.212	23.017	-7.370	1.00	27.53
9131	0		В	314	13.045	23.018	-6.148		27.94
9132	OXT		В	314	14.311	22.729	-7.848		26.55
9133	09	ipp			59.879	67.784	6.844		22.62
9134	P7			900	60.281	67.030	8.078		20.44
9135	08	ipp			61.128	65.793	7.905		20.16
9136	010	ipp		900	58.921	66.747	8.923	1.00	
9137	P11	ipp			58.096	65.364	9.039		20.72
9138	013	ipp			58.271	64.667	7.712		21.48
9139	012			900	58.760	64.598	10.167	1.00	
9140	014	ipp		900	56.677	65.719	9.388	1.00	19.87
9141 9142	06 C5	ipp		900 900	61.085	68.067	9.000	1.00	23.40
9145	C4	ipp ipp		900	60.446 61.386	69.278 70.077	9.396 10.277	1.00	22.55
9148	C2			900	62.729	70.303	9.627		24.00
9149	C3			900	62.729	70.303	8.237		23.48
9153	C1			900	63.818	70.021	10.311		24.77
9156	012				57.820	74.304	11.572		21.28
9157	P9	ris			58.623	73.691	10.433		21.35
9158		ris			58.329	74.511	8.992		22.29
9160		ris			58.206	72.094	10.263		22.10
9162	C8	ris			60.334	73.798	10.791		20.58
9163		ris			61.051	73.167	9.710		21.47
9165		ris			60.832	75.467	10.955		21.49
9166		ris			60.487	76.175	9.664		20.67
9167		ris			60.014	76.127	12.259		20.29
9169	017				62.473	75.654	11.235		16.79
9171	C7			901	60.517	73.036	12.110		20.01
9174	C2			901	61.916	72.843	12.658		20.04

FIGURE 3 (Cont.) DK

Α	В	C	D	E	F	G	H	I	J
9175	C1			901	62.030	72.693	14.038		22.23
9177	C6			901	63.284	72.496	14.614		21.92
9179	C5			901	64.396	72.454	13.790	1.00	
9181	N4			901	64.272	72.597	12.461	1.00	
9182	C3			901	63.073	72.787	11.887	1.00	
9184	09			902	16.064	23.295	-2.975		21.48
9185	P7			902	16.496	22.587	-1.731		20.32
9186	08			902	17.402	21.368	-1.817		20.60
9187	010			902	15.180	22.297	-0.852		19.29
9188	P11			902	14.357	20.933	-0.731		21.41
9189	013			902	14.501	20.303	-2.099		21.14
9190	012			902	15.018	20.139	0.361		19.56
9191	014			902	12.943	21.318			20.18
9192	06			902	17.282	23.658			21.57
9193	C5			902	16.665	24.901			20.59
9196	C4			902	17.539	25.684		1.00	
9199	C2			902	18.923	25.954			20.12
9200	C3			902	19.094	26.613		1.00	20.10
9204	C1			902	19.970	25.641	0.637	1.00	19.72
9207	012			903	13.949	29.944	1.653	1.00	18.96
9208	P9			903	14.827	29.319	0.595	1.00	18.15
9209		ris			14.564	30.066	-0.891	1.00	17.76
9211	010	ris			14.479	27.699	0.371	1.00	17.12
9213	C8		Х	903	16.543	29.484	1.000	1.00	
9214	013			903	17.268	28.905	-0.099	1.00	14.71
9216	P14	ris	Х	903	17.105	31.143	1.147	1.00	16.07
9217	016				16.424	31.703	2.361	1.00	18.08
9218	015	ris	Х	903	18.754	31.239	1.421	1.00	20.15
9220	017			903	16.681	31.883	-0.303	1.00	17.24
9222	C7			903	16.736	28.711	2.310	1.00	15.64
9225	C2			903	18.144	28.461	2.843	1.00	17.89
9226	C1	ris			18.231	28.146	4.193	1.00	17.51
9228	C6	ris	Х	903	19.477	27.908	4.776	1.00	17.87
9230	C5	ris			20.612	27.985	3.980	1.00	18.68
9232	N4	ris	Х	903	20.535	28.281	2.665	1.00	18.45
9233	C3			903	19.332	28.506	2.084	1.00	18.77
9235	MG	MG	Х	904	15.574	31.310	-1.873		21.07
9236		MG		905	17.080	32.751	3.968	1.00	17.94
9237	MG	MG		906	14.279	31.564	2.944	1.00	18.98
9238	MG	MG		907	58.027	75.928	12.811	1.00	21.97
9239		MG	Х		59.508	75.731	8.080	1.00	25.32
9240	MG	MG	Х	909	60.807	77.116	13.792	1.00	19.86
9241	OWO	НОН	Х	1	69.581	70.101	13.536	1.00	18.91
9244		HOH		2	62.678	62.339	10.204	1.00	15.42
9247	OWO			3	25.799	25.747	3.926	1.00	15.73
9250		НОН		4	59.333	62.010	10.213	1.00	18.17
9253		НОН		5	18.822	17.964	0.386	1.00	18.32
9256		нон		6	13.596	24.842	-2.548	1.00	13.98
9259		нон		7	60.443	70.120	5.487	1.00	20.05
9262		НОН		8	67.024	68.022	10.947	1.00	18.31
9265		нон		9	75.891	66.532	13.529	1.00	16.24
9268	OWO	НОН	Х	10	61.389	59.407	28.540	1.00	15.76

FIGURE 3 (Cont.)DL

A	В	С	D	E	F	G	Н	I	J
9271	OWO	нон	х	11	16.713	25.479	-4.403	1.00	16.69
9274	OWO	нон	Х	12	17.228	19.008	-1.948	1.00	17.97
9277	OWO	нон	Х	13	60.948	63.338	7.816	1.00	17.21
9280	OWO	нон		14	12.537	21.690	6.873	1.00	20.29
9283	OWO	нон		15	17.395	34.432	2.680	1.00	15.95
9286	OWO	нон		16	22.715	24.983	3.509	1.00	21.00
9289	OWO	нон		17	23.103	23.679	1.175	1.00	16.66
9292	OWO	нон		18	60.488	77.235	6.934	1.00	16.27
9295	OWO	нон	Х	19	57.327	69.233	7.233	1.00	17.06
9298	OWO	нон	Х	20	15.505	17.649	0.655	1.00	17.89
9301	OWO	нон	Х	21	34.673	22.728	-9.839	1.00	22.21
9304	OWO	НОН	Х	22	12.191	23.940	-0.324	1.00	14.99
9307	OWO	нон	Х	23	4.461	26.280	19.031	1.00	23.20
9310	OWO	нон	Х	24	72.420	88.509	2.009		28.92
9313	OWO	нон	Х	25	73.365	71.690	24.882	1.00	15.83
9316	OWO	нон		26	9.311	27.134	10.014	1.00	16.86
9319	OWO	нон	Х	27	33.303	4.388	14.111	1.00	23.61
9322	OWO	нон		28	9.972	29.039	2.416	1.00	19.40
9325	OWO	нон	Х	29	20.315	24.167	4.178	1.00	21.86
9328	OWO	нон		30	23.161	10.579	20.659	1.00	23.73
9331	OWO	нон		31	62.889	76.521	13.608	1.00	18.10
9334		НОН		32	14.368	17.510	4.944		24.43
9337		нон		33	31.222	26.334	11.934		21.87
9340	OWO			34	17.123	34.428	-0.050	1.00	18.82
9343	OWO			35	65.244	84.346	-6.827	1.00	23.12
9346	OWO	нон		36	53.273	71.292	19.938	1.00	20.38
9349	OWO	нон		37	75.108	70.654	21.698	1.00	19.01
9352	OWO	нон		38	61.370	78.383	15.450	1.00	24.45
9355	OWO	нон		39	64.170	68.585	13.753	1.00	23.11
9358	OWO	нон		40	15.187	3.524	-3.226	1.00	21.48
9361	OWO	нон		41	20.358	39.276	1.884	1.00	22.25
9364	OWO	нон		42	59.729	80.370	3.839		25.41
9367	OWO	нон		43	9.394	25.625	7.660	1.00	19.98
9370	OWO	нон		44	19.279	13.591	19.445	1.00	25.74
9373	OWO	нон	Х	45	18.592	28.894	9.372	1.00	21.52
9376	OWO	нон		46	16.733	32.742	-2.993	1.00	17.70
9379	OWO	нон	Х	47	28.337	35.553	9.793	1.00	24.55
9382		нон		48	71.766	52.024	1.660		25.10
9385		нон		49	5.509	18.812	21.857		25.11
9388	OWO	нон	Х	50	25.249	44.467	-11.635		22.90
9391		нон		51	16.089	35.932	-5.867		20.15
9394		нон		52	50.870	75.101	10.886		22.51
9397		нон		53	58.111	59.051	3.773		23.52
9400		нон		54	84.343	49.350	23.069		19.58
9403		нон		55	56.087	75.553	13.615		15.17
9406		нон		56	19.494	34.654	-1.382		20.86
9409		нон		57	8.799	19.400	4.773		21.44
9412		нон		58	39.726	12.512	12.694	1.00	37.61
9415		нон		59	12.786	3.396	7.777		28.21
9418		нон		61	33.547	28.085	-16.167		24.17
9421		нон		62	60.548	68.421	32.431		22.66
9424		нон		63	52.652	63.594	14.580		21.16

FIGURE 3 (Cont.) DM

A	В	С	D	E	F	G	Н	I	J
9427	OWO	нон	х	64	63.267	78.956	8.228	1.00	23.96
9430		нон		65	21.674		-16.591	1.00	19.82
9433	OWO	нон	Х	66	62.524	73.265	19.235	1.00	24.72
9436	OWO	нон	Х	67	50.175	67.476	14.681	1.00	24.07
9439		HOH		68	16.317	24.542	22.592	1.00	24.88
9442	OWO	НОН	Х	70	13.596	32.913	1.425	1.00	18.95
9445	OWO	нон	X	71	33.743	4.683	-9.292	1.00	21.88
9448	OWO	НОН	X	72	84.877	52.105	15.691	1.00	35.89
9451		HOH		73	28.069	7.721	-7.921	1.00	22.28
9454		нон		74	29.256	1.053	13.166	1.00	28.61
9457		НОН		75	26.790	-1.137	5.597	1.00	33.71
9460		нон		76	33.840	27.398	-6.991	1.00	
9463		НОН		77	20.039	38.545	-21.843	1.00	
9466		нон		78	49.910	55.142	25.447	1.00	26.46
9469		нон		79	9.843	14.477	-1.615	1.00	
9472		НОН		80	36.808	16.350	8.648		22.19
9475 9478		HOH		81	43.245	14.999	0.753		22.13
9478		HOH HOH		82 83	57.361	79.956	11.239	1.00	25.78
9484		НОН		84	9.775 68.131	24.342 69.501	-1.506 22.346	1.00	
9487		нон		85	64.173	83.689	11.530	1.00	28.17 19.53
9490		нон		86	58.920	48.042	6.438	1.00	
9493		нон		87	57.493	77.168	11.232	1.00	19.16
9496		нон		88	77.326	71.627	2.643	1.00	
9499		нон		89	74.547	71.580	7.451	1.00	
9502		нон		91	48.469	59.380	21.046	1.00	23.24
9505		нон		92	59.723	83.049	3.647		26.08
9508		нон		93	29.853	24.288	-1.800	1.00	33.40
9511	0	нон	Х	94	56.128	56.547	-0.069	1.00	31.76
9514	0	HOH	Х	95	60.992	57.155	5.055	1.00	25.17
9517	0	HOH	Х	96	57.412	60.876	1.767	1.00	27.49
9520	0	HOH	Х	98	10.425	34.341	14.720	1.00	25.28
9523	0	HOH	X	99	58.393	61.924	14.465	1.00	21.57
9526	0	нон		100	15.514	40.203	-8.447	1.00	25.83
9529	0	нон		101	71.395	44.872	6.706	1.00	23.21
9532	0	НОН		102	59.088	84.453	1.416	1.00	21.13
9535	0	нон		103	10.805	35.476	2.484	1.00	30.21
9538	0	НОН			78.675	67.094	-0.168		30.94
9541	0	HOH			53.216	69.834	17.573		21.88
9544	0			106	11.540	21.193	-2.775		23.63
9547 9550	0	HOH HOH			56.434	66.036	16.603 8.469		21.18
9553	0			109	53.589 22.171	69.002 2.588	12.364		26.03 25.07
9556	0	нон			77.332	49.094	0.357		25.35
9559	Ö	нон			33.771	36.319	-2.063		30.82
9562	Ö	нон			12.214	37.251	-5.519		20.62
9565	ō	НОН			68.012	47.978	18.112		22.53
9568	0	нон			52.583	66.344	14.741		24.60
9571	0	нон			54.317	78.524	24.510		28.76
9574	0	нон			17.315	3.665	4.180		31.96
9577	0	нон	Х	117	41.900	14.903	-5.570	1.00	23.73
9580	0	нон	Х	118	25.232	6.606	-7.167	1.00	24.37

FIGURE 3 (Cont.) DN

Α	В	С	D	E	F	G	H	Ι	J
9583	0	нон	х	119	69.198	51.022	2.442	1.00	32.30
9586	0	нон	Х	120	54.454	75.970	7.898		29.61
9589	0	нон	Х	121	72.835	54.092	-0.028		28.37
9592	0	нон			13.624	16.407	-7.904		26.27
9595	0	нон			52.606	51.548	23.966		31.75
9598	0	нон		124	64.545	60.261	-5.452		26.24
9601	ō	нон			48.485	73.411	29.403		35.53
9604	ō	НОН			73.394	45.286	22.697		31.73
9607	Ō	НОН			1.619	16.387	23.748		35.87
9610	ō	нон			51.331	52.037	31.882		32.80
9613	0	нон			59.702	84.785	5.880		28.09
9616	ō			131	35.875	32.733	-2.230		41.90
9619	ō	нон			56.078	68.294	9.410		23.25
9622	ō	НОН			68.940	88.925	-1.936		24.65
9625	ō	НОН			66.234	47.041	21.983		27.75
9628	Ö	нон			61.333	46.476	6.833		25.98
9631	ō	нон			67.556	54.792	30.084		27.45
9634	Ö	нон			40.092	4.846	14.202		33.56
9637	Ö	НОН			6.434	23.324	4.635		23.23
9640	ō	нон			53.326	52.199	10.569		27.46
9643	Ö	НОН			16.797	40.699			31.25
9646	Ö	нон			55.505	68.569	5.472		31.05
9649	Ö	нон			19.829	28.141	-14.550		32.03
9652	ō	нон		143	72.192	80.036	19.386		26.69
9655	ō	НОН			49.567	62.818	10.675		36.36
9658	ō	НОН			77.624	80.795	7.572		30.84
9661	0	НОН		146	70.251	84.697	14.333		29.10
9664	ō	нон			22.147	28.439			25.06
9667	0	нон			13.634	35.572	1.265		25.62
9670	0	нон			82.244	46.629	23.769		35.68
9673	0	нон			63.846	88.990	3.561		28.36
9676	0	нон			64.405	73.293	-9.004		59.74
9679	0	нон			19.585	44.233	-0.968		31.22
9682	0	нон			17.128	12.637	-4.589		25.38
9685	0	нон			5.113	33.908	7.713		38.08
9688	0	нон	х	156	30.306	34.937	-7.899		34.44
9691	0	нон			3.129	22.986	-4.541		39.21
9694	0	нон			66.626	69.399	13.372		23.00
9697	0			159	63.446	57.641	29.205		27.23
9700	0	нон			54.243	50.317	14.175		34.68
9703	0	HOH	Х	161	66.368	78.182	-9.856		26.10
9706	0	нон			53.159	57.048	10.179		27.95
9709	0	нон	Х	163	44.219	16.007	-6.192		25.11
9712	0	нон	Х	164	80.589	61.008	18.291		25.88
9715	0	нон			28.989	38.706	2.563		25.75
9718	0	HOH	Х	166	11.238	30.773	0.615		24.14
9721	0	нон	Х	167	53.608	73.127	12.234		26.24
9724	0	нон	Х	169	63.586	45.033	14.349		31.13
9727	0	НОН	Х	170	77.596	48.785	23.097		26.73
9730	0	нон	X	171	84.848	48.026	14.304		29.46
9733	0	нон	X	172	4.265	15.315	11.290	1.00	29.33
9736	0	нон	Х	173	3.381	31.069	16.737	1.00	33.72

FIGURE 3 (Cont.)DO

Α	В	С	D	E	F	G	Н	I	J
9739	0	нон	Х	174	55.238	65.487	7.142	1.00	31.03
9742	0	нон	Х	175	9.341		-11.288		29.49
9745	0	нон			53.199	53.483	20.584		32.49
9748	0	нон	Х	177	14.338	14.643	-5.988		23.99
9751	0	нон	Х	178	38.329		-11.565		45.14
9754	0	нон	Х	179	39.337	18.256	2.081	1.00	27.57
9757	0	нон	Х	180	56.191	81.845	4.467	1.00	30.98
9760	0	нон	Х	181	20.859	16.036	-15.248	1.00	24.19
9763	0	нон	Х	182	52.592	52.636	34.412	1.00	33.36
9766	0	нон	X	183	8.751	22.025	4.991	1.00	21.08
9769	0	НОН	X	184	63.183	88.654	8.668	1.00	32.88
9772	0	нон	Х	185	23.296	39.123	11.088	1.00	28.53
9775	0	нон		186	21.029	42.374	-4.623	1.00	40.24
9778	0	нон		187	61.193	73.706	-5.808	1.00	35.26
9781	0	НОН		188	55.468	47.798	19.949	1.00	28.75
9784	0	НОН		189	35.734	28.370	-1.891		42.91
9787	0	нон		190	28.941	9.752	-9.745	1.00	28.83
9790	0	нон		191	60.836	85.243	-5.478	1.00	33.63
9793	0	нон		193	85.606	61.921	11.265	1.00	33.58
9796	0	нон		194	78.387	74.119	-1.722	1.00	50.78
9799	0	нон		195	7.183	30.679	0.916	1.00	33.15
9802	0	нон		196	32.652	28.076	-18.831		28.06
9805	0	нон		197	53.948	51.530	21.729	1.00	30.16
9808	0	нон		198	3.740	12.442	13.203	1.00	38.10
9811	0	нон		199	81.671	47.299	9.794	1.00	39.29
9814	0	нон			76.149	46.441	21.909	1.00	32.74
9817	0	нон			61.151	42.663	13.748		62.81
9820 9823	0	НОН			54.688	79.719	12.391	1.00	30.29
9826	0	НОН НОН			51.275	79.190 30.823	10.957	1.00	40.83
9829	0	НОН		205	14.506 14.195	30.823	-3.503 -1.332	1.00	21.42 19.33
9832	Ö	НОН			12.434	31.396	3.683	1.00	16.08
9835	Ö	нон			18.969	32.213	3.765	1.00	20.53
9838	Ö	нон			17.536	34.005	5.600	1.00	16.75
9841	Ö	нон			33.461	39.878	0.879		48.09
9844	Ö	НОН			78.263	66.876	16.527	1.00	37.29
9847	Ō	нон			80.975	67.293	15.894	1.00	39.50
9850	0	нон			82.405	67.613	13.856		46.74
9853	0	нон			50.671	57.527	11.069		40.42
9856	0	нон			51.601	55.517	13.513		33.26
9859	0	HOH	Х	215	62.729	54.517	30.771		40.62
9862	0	HOH	Х	216	60.331	52.329	31.300	1.00	52.01
9865	0	нон	Х	217	31.078	32.997	-9.951	1.00	29.54
9868	0	нон	Х	218	33.614	33.829	-1.558	1.00	23.66
9871	0	нон	X	219	3.882	31.855	12.746		38.99
9874	0	нон			15.840	40.330	-3.855		26.18
9877	0	нон			15.995	38.459	-6.211		24.53
9880	0	нон			63.555	73.039	-4.552		36.76
9883	0	нон			65.686	72.948	-6.046		30.87
9886	0	нон			61.071	89.367	2.768		33.44
9889	0	нон			85.368	50.306	25.290		39.68
9892	0	нон	Х	226	10.770	31.661	-1.862	1.00	30.59

FIGURE 3 (Cont.)DP

A	В	С	D	E	F	G	H	I	J
0005	_	***	٠,	005	68.084				
9895	0	НОН			67.074	86.090			47.90
9898	0	НОН			72.225	82.393			28.15
9901 9904	0	нон нон			23.258	30.948			37.49
9904	0				18.514	43.214			25.15
9910	0	нон нон			18.316	39.793			30.27
9913	0	НОН			18.565 10.124	22.994	-20.157		27.88
9916	0	НОН			40.682				22.65
9919	0	НОН			60.087	5.559 44.060			35.43 29.04
9922	0	НОН			65.753	46.800	7.813 19.256		33.55
9925	o	нон			47.350	74.880	26.880		40.56
9928	Ö	нон			48.590	70.295			22.47
9931	Ö	НОН			62.111	62.571			41.29
9934	Ö	нон			58.266	75.096			20.97
9937	ō	нон			57.930	77.196	8.555		21.06
9940	Ö	нон			60.766	78.814	9.905		24.54
9943	ō	нон			61.087	78.751	12.516		17.96
9946	ō	НОН			66.063	45.873	5.892		30.86
9949	Ō	НОН			68.834	44.595	6.140		27.12
9952	0	нон			40.240	21.104	-0.696		29.77
9955	0	нон			54.038	67.321	16.979		23.18
9958	0	нон			6.161	36.828	-2.610		45.75
9961	0	нон	Х	249	32.414	42.931	-5.770		26.20
9964	0	HOH	Х	250	8.263	18.675	-2.300		37.46
9967	0	нон	Х	251	57.682	88.576	6.524		41.67
9970	0	НОН	Х	252	9.403	38.851	14.485	1.00	38.72
9973	0	НОН	Х	253	7.150	40.262	16.390	1.00	45.72
9976	0	HOH	Х	254	53.657	64.735	-1.870	1.00	50.87
9979	0	нон			54.909	49.982	11.303	1.00	29.97
9982	0	нон			54.469	48.142	15.766		35.94
9985	0	нон			64.819	51.877	25.591	1.00	48.64
9988	0	HOH			48.466	60.211	34.761	1.00	34.69
9991	0	нон			50.594	60.418	33.231		29.29
9994	0	НОН			44.303	61.380	23.666		50.60
9997	0	нон			42.915	58.238	26.279		44.44
10000	0	НОН			52.554	63.196	6.954		45.59
10003	0	HOH			75.789	43.073	11.027		45.52
10006	0	HOH				46.831			38.28
10009 10012	0	HOH			44.196	64.994	15.827		37.65
10012	0	HOH			43.951	62.363	16.102		46.48
10013	0	нон нон			39.222	63.891	21.996		52.12
10018	0	НОН			42.850 48.526	63.664 74.293	23.396 31.675		50.80
10021	Ö	НОН			67.670	48.672	31.258		36.34 51.39
10027	Ö	НОН			81.199	48.984	16.751		28.66
10027	o	НОН			79.911	47.943	14.775		31.46
10033	Ö	НОН			85.017	50.279	19.126		30.80
10036	Ö	нон			64.657	81.303	10.384		30.96
10039	ō	нон			62.329	87.607	6.341		31.55
10042	0	нон			64.640	86.808	5.080	1.00	
10045	0	нон			60.179	93.225	8.295	1.00	
10048	0	нон	X	278	73.593	79.168	1.381		35.41

FIGURE 3 (Cont.)DQ

Α	В	C	D	E		F	G	H	I	J
	_									
10051	0			279	74.		77.325	-0.481		41.75
10054	0			280	77.		76.446	0.836		38.59
10057	0			281	74.		76.085	-2.785	1.00	
10060	0	нон			79.		78.702	16.390	1.00	
10063	0	нон			77.		76.993	10.420		32.78
10066	0	нон			77.		78.246	8.067		37.50
10069	0	нон			73.		68.872	7.682		33.72
10072	0	нон			77.		62.256	8.543		45.53
10075	0			287	84.		47.863	10.649		33.57
10078	0	нон			89.		59.221	10.145		51.60
10081	0			289	88.		58.568	7.606		57.77
10084	0			290	44.		73.834	1.582		48.13
10087	0			291	49.		81.495	7.222		45.30
10090	0	НОН			70.		68.660	-8.004		41.08
10093	0	НОН			81.		67.174	-2.963		39.74
10096	0	НОН			77.		57.817	-5.855		32.90
10099	0			295	76.		60.286	-6.405		33.62
10102	0			296	72.		51.978	-1.088		40.76
10105	0			297	69.		55.952	-6.441		41.52
10108	0			298	66.		60.092	-7.585		37.64
10111	0			299	58.		67.727	-7.779		45.55
10114	0			300	13.		3.105	-5.157		38.92
10117	0			301	13.	794	2.664	-0.805	1.00	33.87
10120	0			302		442	1.396	0.758		53.73
10123	0			303	17.	525	-0.047	0.589	1.00	35.96
10126	0			304	13.	277	5.297	-9.056		41.07
10129	0			305		451	8.808	-4.245		33.55
10132	0			306		127	5.641	1.860		28.72
10135	0			307	17.		2.139	-2.799		30.54
10138	0			308		535	2.393	-4.513		33.31
10141	0			309		312	12.628	0.396	1.00	37.60
10144	0			310		665	11.510	3.549	1.00	34.31
10147	0			311		051	11.080	6.071	1.00	
10150	0			312		116	7.158	11.883	1.00	
10153	0			313		385	9.324	10.796	1.00	
10156	0			314		622	2.412	13.739	1.00	31.45
10159	0			315		037	2.160	16.038	1.00	
10162	0			316		930	10.969	15.786		34.44
10165	0			317		581	9.801	22.907		46.13
10168	0			318		584	18.885	-1.559		52.72
10171	0			319	37.		2.115	-2.954		43.48
10174	0			320	36.		3.493	-6.561		45.09
10177	0			321	20.		0.677	4.712		26.47
10180	0			322	20.		8.134	16.042	1.00	
10183	0			323	19.		10.262	18.888		37.59
10186	0			324	24.		25.499	12.581	1.00	
10189 10192	0			325	14.		39.048	7.973		31.76
				326		756 810	39.045 36.884	9.415		50.88
10195 10198	0			327 328		242	25.497	3.543 -3.703		29.56
10198	0			329		219	33.875	16.266		46.56
10201	0			330		544	29.687	13.872		40.23
10207	9	поп	11	550	1.	J 1 1	25.007	13.072	1.00	10.23

FIGURE 3 (Cont.) DR

Α	В	С	D	E	F	G	H	I	J
	_								
10207	0			331	-0.474		15.144		54.89
10210	0			332	4.337		19.199		36.94
10213	0	нон			-1.539				45.30
10216	0	нон			-2.107		12.397		38.86
10219	0	НОН			2.398				43.49
10222	0			336	4.084		25.067		35.34
10225	0			337	3.978				45.80
10228	0			338	3.094				40.72
10231	0			339	4.241				35.53
10234	0			340	37.329				35.31
10237	0			341	39.684				27.65
10240	0			342	36.317				40.32
10243 10246	0			343	32.070			1.00	
10246	0			344 345	32.703				30.65
10249	0			346	21.195 26.360				23.85
10252	0			347	23.190				37.57 34.90
10258	0			348	18.440				34.50
10250	0			349	15.607		-4.850		31.05
10264	0			350	13.692				41.66
10267	Ö			351	31.128				41.41
10270	Ö			352	31.689		-4.627		30.20
10273	Ö	нон			32.993		-3.190		38.18
10276	ō			354	27.426				33.92
10279	ō	нон			43.796		3.108		23.99
10282	o			356	42.070				30.43
10285	Ō			357	43.287				33.75
10288	0			358	39.828				35.08
10291	0			359	38.165				37.82
10294	0			360	33.950				45.50
10297	0	нон	Х	361	11.762		-4.528	1.00	31.90
10300	0	нон	Х	362	3.975	32.061	-8.760	1.00	36.38
10303	0	нон	Х	363	15.528	42.830	-7.772	1.00	35.25
10306	0	нон	X	364	14.500	29.223	-15.075	1.00	41.38
10309	0	нон	Х	365	32.850	21.982	-18.707	1.00	37.44
10312	0			366	40.592	8.573	-5.209	1.00	37.21
10315	0			367	25.811				30.06
10318	0	НОН	Х	368	26.945	13.028	-17.719	1.00	49.20
10321	0	нон	Х	369	24.479		-17.748		49.87
10324	0	HOH	Х	370	21.021	. 17.997	-19.491		46.80
10327	0	нон	Х	371	23.217	19.367	-20.360		51.32
10330	0			372	22.674				43.41
10333	0			373	12.811				35.30
10336	0			374	55.709				47.10
10339	0			375	54.100				43.29
10342	0			376	48.970		17.748		39.82
10345	0	нон			41.899				46.67
10348	0			378	48.368				30.58
10351	0			379	48.070				35.54
10354 10357	0			380 381	47.998				42.38
10357	0			381	50.349				39.16
T0200	J	HOH	Λ	302	32.392	20.723	0.642	1.00	35.35

FIGURE 3 (Cont.) DS

Α	В	С	D	E	F	G	H	I	J
10363	0	нон	х	383	30.720	27.097	-2.250	1.00	27.18
10366	0	НОН	Х	384	37.015	26.821	2.778		49.37
10369	0	нон	Х	385	38.443	23.443	3.534		33.87
10372	0	HOH	Х	386	38.669	19.697	6.394	1.00	36.31
10375	0	HOH	Х	387	30.186	-3.337	5.179	1.00	43.04
10378	0	HOH	Х	388	36.379	2.179	1.556	1.00	42.15
10381	0	HOH	Х	389	41.111	3.324	0.448	1.00	36.90
10384	0	HOH	Х	390	43.161	2.676	-1.085	1.00	38.66
10387	0	HOH	Х	391	62.047	69.399	25.389	1.00	88.66
10390	0	HOH	Х	392	64.141	69.344	27.823	1.00	41.19
10393	0	HOH	Х	393	58.875	89.405	12.710	1.00	64.96
10396	0	HOH	Х	394	52.351	74.162	-4.548	1.00	47.29
10399	0	HOH	Х	395	53.730	70.282	-5.715	1.00	55.71
10402	0	HOH			47.666	76.863	1.325	1.00	34.63
10405	0	НОН			59.660	75.843	-9.785	1.00	41.09
10408	0	HOH			62.561	78.886	-9.940	1.00	50.51
10411	0	HOH	Х	399	30.260	2.431	-11.763	1.00	34.80
10414	0	HOH	Х	400	27.528	3.971	-14.875	1.00	45.91
10417	0	HOH			33.506	13.418	-15.971		38.77
10420	0	HOH			41.028	6.141	-7.128		49.46
10423	0	нон			28.710		-18.837		26.44
10426	0	нон			29.796		-15.688		37.98
10429	0	нон			27.243		-15.645		37.96
10432	0	нон			31.047	35.920			55.58
10435	0	нон			33.680	38.851	-7.405		50.01
10438	0	нон			25.402	37.066	-19.531		37.00
10441	0	нон			35.153	33.776	5.764		48.02
10444	0	нон			35.151	34.064	2.494		34.05
10447	0	НОН			34.154	30.349	7.013		44.18
10450	0	НОН			8.762	37.486	1.397		38.43
10453	0	НОН			7.201	35.165	1.535		41.39
10456	0	НОН			26.384	40.391	4.437		36.18
10459	0	нон			51.309	51.810	-0.301		39.62
10462	0	нон			29.679	4.776	17.263		29.29
10465	0	нон			28.029	5.806	20.001		42.73
10468	0	нон			20.603	24.902	18.280		45.48
10471	0	нон			56.231	57.185	2.974		32.25
10474	0	нон			53.164	57.686	5.692		35.05
10477	0	HOH	Х	421	65.428	51.862	28.325	1.00	40.33